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Q Exactive GC and Exactive GC

Mass Spectrometers

Operating Manual

1R120706-0002 Revision C June 2018



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Release History: Revision A released in June 2015. Revision B released in July 2016. Revision C released in June 2018.

Contacting Us

There are several ways to contact Thermo Fisher Scientific.

Assistance

For technical support and ordering information, please visit:

https://gcgcms.freshdesk.com/support/home

Service contact details are available under:

www.unitylabservice.com

For brochures, application notes and other material, please visit:

www.thermofisher.com

For operating manuals, please contact your local Service organization.

Suggestions to the Manual

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United States

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- You are encouraged to report errors or omissions in the text or index. Thank you.

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Chapter 1 Using this Manual

Welcome to the Thermo Scientific[™] Q Exactive[™] GC or Exactive GC system! The Q Exactive GC and Exactive GC systems are members of the Thermo Scientific family of mass spectrometer (MS) detectors that are powered by Orbitrap[™] technology.

Thermo Scientific Q Exactive GC and Exactive GC instruments are designed to be placed on a bench in the laboratory and come with an ExtractaBrite[™] removable ion source cartridge, a quadrupole mass filter for precursor ion selection, and a collision cell for performing MS/MS experiments.

- "About This Manual" on page 1-2
- "Typographical Conventions" on page 1-3
- "Reference Documentation" on page 1-5

About This Manual

This *Q Exactive GC and Exactive GC Operating Manual* contains precautionary statements that can prevent personal injury, instrument damage, and loss of data if properly followed. It also describes the modes of operation and principle hardware components of your Exactive Series instrument. In addition, this manual provides step-by-step instructions for cleaning and maintaining your instrument.

Designed, manufactured and tested in an ISO9001 registered facility, this instrument has been shipped to you from our manufacturing facility in a safe condition.

This instrument must be used as described in this manual. Any use of this instrument in a manner other than described here may result in instrument damage and/or operator injury.

Typographical Conventions

| | This section describes typographical conventions that have been established for Thermo Fisher Scientific manuals. |
|-----------------------|--|
| Signal Word | |
| | Make sure that you follow the precautionary statements presented in this manual. The special notices appear different from the main flow of text: |
| | NOTICE Points out possible material damage and other important information in connection with the instrument. ▲ |
| Viewpoint Orientation | |
| | The expressions <i>left</i> and <i>right</i> used in this manual always refer to the viewpoint of a person that is facing the front side of the instrument. |
| Data Input | |
| | Throughout this manual, the following conventions indicate data input and output with the computer: |
| | • Messages displayed on the screen are represented by capitalizing the initial letter of each word and by italicizing each word. |
| | • Input that you enter by keyboard is identified by quotation marks: single quotes for single characters, double quotes for strings. |
| | • For brevity, expressions such as "choose File > Directories " are used rather than "pull down the File menu and choose Directories." |
| | • Any command enclosed in angle brackets < > represents a single keystroke. For example, "press <f1></f1> " means press the key labeled <i>F1</i> . |
| | • Any command that requires pressing two or more keys simultaneously is shown with a plus sign connecting the keys. For example, "press <shift></shift> + <f1></f1> " means press and hold the <shift> key and then press the <f1> key.</f1></shift> |
| | • Any button that you click on the screen is represented in bold face letters. For example, "click Close ". |

Topic Headings

The following headings are used to show the organization of topics within a chapter:

Chapter 1 Chapter Name

Second Level Topics

Third Level Topics

Fourth Level Topics

Reference Documentation

This *Q Exactive GC and Exactive GC Operating Manual* represents the Original Operating Instructions. In addition to this manual, Thermo Fisher Scientific provides other documents for the Q Exactive GC mass spectrometer that are not part of the Original Operating Instructions. Reference documentation for the Q Exactive GC system includes:

- Q Exactive GC and Exactive GC Preinstallation Requirements Guide
- Q Exactive GC Software Manual
- *Q Exactive GC QuickStart Guide*

Reference documentation for the Exactive GC system includes:

- Q Exactive GC and Exactive GC Preinstallation Requirements Guide
- Exactive GC Software Manual
- Exactive GC QuickStart Guide

You can access PDF files of the documents listed above and of this manual from the data system computer. The software also provides Help.

* To view product manuals

Go to Start > All Programs > Thermo Exactive Series > Manuals.

A printed version of this *Q Exactive GC and Exactive GC Operating Manual* is shipped with the instrument. A printed version of the *Q Exactive GC and Exactive GC Preinstallation Requirements Guide* is part of the Preinstallation Kit. This kit is sent to your laboratory before the arrival of the mass spectrometer.

NOTICE If this manual is in a language other than English: Translations of the above documents that are available in this language are shown with their titles translated and the English title in parentheses. See "Contacting Us" at the beginning of this manual for information about obtaining current manuals. ▲

Refer also to the user documentation provided by the manufacturers of third-party components:

- Forepump
- Turbomolecular pumps
- Data system computer and monitor
- Safety data sheets

Chapter 2 Scope of Delivery

This chapter lists she standard components of your Q Exactive GC or Exactive GC GC/MS system and optional components.

Contents

- "Standard System Components" on page 2-1
- "Optional System Components" on page 2-2

Standard System Components

A Q Exactive GC or Exactive GC standard system comprises the following components:

- Q Exactive GC or Exactive GC mass spectrometer
- Thermo Scientific[™] TRACE[™] 1310 gas chromatograph (GC)
- Data system computer with monitor
- Forepump and drip pan for forepump
- Installation Kit including
 - Equipment for connecting the above components (hoses, cables)
 - Computer equipment
 - Tools for installation and maintenance
 - Spare parts
- Printed manual
 - Q Exactive GC and Exactive GC Operating Manual

In addition to this printed manual, other documents for the mass spectrometer are available as PDF files on the data system computer. See "Reference Documentation" on page 1-5 for a list.

Optional System Components

For reference, the following list contains components that are frequently shipped with the standard Q Exactive GC or Exactive GC GC/MS system. They are not part of the standard system and may therefore not be present in your laboratory:

• Thermo Scientific[™] TriPlus[™] RSH autosampler

Chapter 3 Functional Description

This chapter provides an overview of the functional elements of a Q Exactive GC and Exactive GC mass spectrometer.

- "General Description" on page 3-2
- "Control Elements" on page 3-7
- "Ion Optics of the Q Exactive GC Mass Spectrometer" on page 3-14
- "Ion Optics of the Exactive GC Mass Spectrometer" on page 3-15
- "Curved Linear Trap" on page 3-21
- "Orbitrap Analyzer" on page 3-22
- "HCD Cell" on page 3-25
- "Vacuum System" on page 3-26
- "Cooling Fans" on page 3-29
- "Gas Supply" on page 3-30
- "Printed Circuit Boards" on page 3-32

General Description

Q Exactive GC and Exactive GC mass spectrometers are stand-alone Orbitrap[™] instruments with an extractable ion source for gas chromatography (GC) mass spectrometry (MS) high-throughput applications. The instruments are designed to be placed on a bench in the laboratory. This chapter describes the principal components of Q Exactive GC and Exactive GC systems and their respective functions.

Layout of the Q Exactive GC Mass Spectrometers

The Q Exactive GC mass spectrometer consists of the main components listed here:

- Ion source that is removable under vacuum
- Quadrupole mass filter for precursor ion selection
- Intermediate storage device (C-Trap) for short pulse injection
- Collision cell for performing HCD (Higher Energy Collisional Dissociation) experiments
- Orbitrap analyzer for Fourier transform mass analysis

Figure 3-1 shows a front view of the Q Exactive GC MS. For a schematic view of the instrument layout, see Figure 3-7 on page 3-14.



Figure 3-1. Q Exactive GC MS front view

Operating Modes of the Q Exactive GC MS

Samples can be introduced into the TRACE 1310 GC manually or by using an autosampler. See the GC and autosampler user manuals for instructions on injecting samples.

The quadrupole rod assembly operates as ion transmission device with the possibility to filter the transmitted ions according to their mass-to-charge ratios. By applying RF and DC voltages to the rods, the filter characteristic is configured. See "Quadrupole Mass Filter" on page 3-18 for details.

The ions are transferred into the C-Trap through three stages of differential pumping. See "Ion Optics of the Q Exactive GC Mass Spectrometer" on page 3-14 for details. In the C-Trap, the ions are accumulated and their energy is dampened using a bath gas (nitrogen). The ions are then injected through three further stages of differential pumping using a lens system (Z-lens) into the Orbitrap analyzer where mass spectra are acquired by image current detection. The vacuum inside the Orbitrap analyzer is maintained below 1E-9 mbar. See "Orbitrap Analyzer" on page 3-22 for details.

Ions are passed through the C-Trap into the HCD cell. The HCD cell adds a Higher Energy Collision Induced Dissociation capability to the instrument. In combination with the quadrupole mass filter this allows MS/MS experiments or all-ion fragmentation (AIF) in case of a broad range of selected mass-to-charge ratios. After the ions have been fragmented in the HCD cell, the HCD cell voltages are ramped up and the ions are transferred back into the C-Trap from where they are injected into the Orbitrap analyzer for detection. See page 3-25 for a description of the HCD cell.

| Table 3-1. | Measuring | properties | of the | Q Exactive | GC |
|------------|-----------|------------|--------|------------|----|
|------------|-----------|------------|--------|------------|----|

| Mass Range for Full Scans | m/z 50–3000 (Scan range: last mass ≤ 15 × first mass) |
|---------------------------|---|
| Precursor Ion Selection | |
| $50 < m/z \le 400$ | Any isolation widths between 0.4 amu and full scan |
| $400 < m/z \le 700$ | Any isolation widths between 0.7 amu and full scan |
| $700 < m/z \le 1000$ | Any isolation widths between 1.0 amu and full scan |
| $1000 < m/z \le 2000$ | Any isolation widths between 2.0 amu and full scan |
| $2000 < m/z \le 2500$ | Any isolation widths between 3.0 amu and full scan |
| 2500 < m/z | No precursor ion isolation |
| Mass Resolution | 15000 at <i>m/z</i> 200 at a scan rate of 18 Hz 30000 at <i>m/z</i> 200 at a scan rate of 12 Hz 60000 at <i>m/z</i> 200 at a scan rate of 7 Hz 120000 at <i>m/z</i> 200 at a scan rate of 3 Hz |
| Mass Accuracy | <3 ppm with external calibration (under defined conditions) <1 ppm using internal standard, lock masses (under defined conditions) |
| Polarity Switching | One full cycle in < 1 sec (one full scan positive mode and one full scan negative mode at resolution setting of 60000) |
| Dynamic Range | >5000 within a single scan |

Layout of the Exactive GC Mass Spectrometers

The Exactive GC mass spectrometer consists of the main components listed here:

- Ion source that is removable under vacuum
- Quadrupole mass filter for SIM ion selection
- Intermediate storage device (C-Trap) for short pulse injection
- Orbitrap analyzer for Fourier transform mass analysis

Figure 3-1 shows a front view of the Exactive GC MS. For a schematic view of the instrument layout, see Figure 3-7 on page 3-14.



Figure 3-2. Exactive GC MS front view

Operating Modes of the Exactive GC MS

Samples can be introduced into the TRACE 1310 GC manually or by using an autosampler. See the GC and autosampler user manuals for instructions on injecting samples.

The quadrupole rod assembly operates as ion transmission device with the possibility to filter the transmitted ions according to their mass-to-charge ratios. By applying RF and DC voltages to the rods, the filter characteristic is configured. See "Quadrupole Mass Filter" on page 3-18 for details.

The ions are transferred into the C-Trap through three stages of differential pumping. See "Ion Optics of the Q Exactive GC Mass Spectrometer" on page 3-14 for details. In the C-Trap, the ions are accumulated and their energy is dampened using a bath gas (nitrogen). The ions are then injected through three further stages of differential pumping using a lens system (Z-lens) into the Orbitrap analyzer where mass spectra are acquired by image current detection. The vacuum inside the Orbitrap analyzer is maintained below 1E-9 mbar. See "Orbitrap Analyzer" on page 3-22 for details.

| Mass Range for Full Scans | m/z 50–3000 (Scan range: last mass $\leq 15 \times \text{first mass}$) |
|----------------------------|--|
| SIM Ion Selection | |
| $50 < m/z \le 400$ | Any isolation widths between 0.4 amu and full scan |
| $400 < m/z \le 700$ | Any isolation widths between 0.7 amu and full scan |
| $700 < m/z \le 1000$ | Any isolation widths between 1.0 amu and full scan |
| $1000 < m/z \le 2000$ | Any isolation widths between 2.0 amu and full scan |
| $2000 < m/z \le 2500$ | Any isolation widths between 3.0 amu and full scan |
| 2500 < <i>m</i> / <i>z</i> | No SIM ion isolation |
| Mass Resolution | 15000 at <i>m/z</i> 200 at a scan rate of 18 Hz 30000 at <i>m/z</i> 200 at a scan rate of 12 Hz 60000 at <i>m/z</i> 200 at a scan rate of 7 Hz |
| Mass Accuracy | <3 ppm with external calibration (under defined conditions) <1 ppm using internal standard, lock masses (under defined conditions) |
| Polarity Switching | One full cycle in < 1 sec (one full scan positive mode and one full scan negative mode at resolution setting of 60000) |
| Dynamic Range | >5000 within a single scan |

Table 3-2. Measuring properties of the Exactive GC

Control Elements

Q Exactive GC and Exactive GC mass spectrometers are mainly operated from the desktop computer (data system). LEDs at the front side of the instrument give general information about the system status. Switches and ports for other devices of the GC/MS system are located at the power panel on the left side of the instrument. The mains inlet and the Ethernet port are located at the rear side of the instrument. This section describes the control elements for important system functions.

System Status LEDs

Five system status LEDs at the front side (See Figure 3-3.) indicate main functions of the system. They are controlled by the source board (See page 3-33.). Table 3-3 explains the function of the LEDs.



| Figure | 3-3. | System status LEDs |
|--------|------|--------------------|
| | | 1 |

| | eyotom otatao EEDo of the | |
|----------|---------------------------|--|
| LED | Status | Information |
| Power | Green | Main power circuit breaker switch on |
| | Off | Main power circuit breaker switch off |
| Vacuum | Green | Operating vacuum reached |
| | Yellow | Vacuum insufficient for measurements, RF can be switched on ^a |
| | Green/Yellow flashing | System bakeout in progress |
| | Off | Vacuum insufficient for measurements, RF cannot be switched on ^a |
| Status | Green | Instrument in operating mode |
| | Yellow | Warn status, does not prevent measurement, however proper operation could be affected ^a |
| | Off | Grave failure detected that does prevent measurement ^a |
| System | Green | System on |
| | Yellow | System in Standby mode |
| | Off | System off |
| Scanning | Blue flashing | Instrument scanning |
| | Off | Instrument not scanning |

Table 3-3. System status LEDs of the Q Exactive GC and Exactive GC mass spectrometer

^a Refer to the Tune software for detailed information about malfunctions of system components.

NOTICE The system status LEDs give a quick overview of the general system status; they do not have any function for the safety status of the instrument. Before performing any maintenance on the instrument, make sure that the main power circuit breaker switch (labeled Main Power) is in the Off (O) position and that the power cords of *mass spectrometer and forepump* are disconnected. It is not sufficient that the Power LED is off because it might be defective. All system status LEDs are off, when the electronics service switch is in the Service Mode position. \blacktriangle

Power Panel

Figure 3-4 shows the rear side of the instrument. Visible are the power panel, power column, forevacuum port, and ventilation slots.

Power Column



Figure 3-4. Rear side of instrument (partial view)

The *main power circuit breaker switch* (labeled Main Power) is located on the power panel at the left side of the mass spectrometer. See Figure 3-5. In the Off (O) position, the circuit breaker removes all power to the mass spectrometer, including the vacuum pumps. In the On (|) position, power is supplied to the mass spectrometer. In the standard operational mode, the circuit breaker is kept in the On (|) position.

NOTICE Power is to remain on. The mass spectrometer should remain on and pumping continuously for optimum performance. ▲

The *electronics service switch* is located on the power panel. See Figure 3-5. In the Service Mode position, the switch removes power to all components of the mass spectrometer except the vacuum system. In the Operating Mode position, power is supplied to all components of the mass spectrometer.

NOTICE The service mode switch does not disable the EI/CI electronics. The EI/CI electronics have a separate switch on the rear. The EI/CI electronics are powered through the power column and will not have power when the main circuit breaker is in the OFF position. ▲



Figure 3-5. Power panel

Both switches contain circuit breakers that protect the electrical wiring of the instrument from an overloaded (overcurrent) condition when it is exposed to more electrical current than it is designed to handle. In case of a thermal overload they interrupt the power supply to the instrument. After cooling down (and removal of the overload), the circuit breakers close and both switches can be used again. If you cannot reset the instrument to the operating mode despite repeated attempts, the circuit breaker inside the switch is blown. In this case, call a Thermo Fisher Scientific field service engineer to replace it.

Peripheral Control

The *peripheral control output* connection allows transmitting *digital* contact closure signals from the mass spectrometer to other devices of the GC/MS system:

• The *Ready Out* port allows the mass spectrometer to provide ready status through contact closure for an external receiving device.

• The *Start Out* port allows the mass spectrometer to provide a programmable contact closure output signal to the inputs of an external receiving device.

NOTICE Refer to the Software Manual or the Tune Help of your instrument for information about setting up contact closure signals.

The contact closure signals are transmitted through a trigger cable that connects the respective port to the external device. A suitable plug connector (P/N 2087270) for the peripheral control output connection is provided with the Installation Kit. See "User I/O Connections" on page 5-16 for specifications of the peripheral control output connection ports.

The *peripheral control input* connection allows transmitting signals from other devices of the GC/MS system to the mass spectrometer:

• The *Start In* port allows the mass spectrometer to start data acquisition upon receiving a *digital* contact closure signal from an external device.

The contact closure signals are transmitted through a trigger cable that connects the respective port to the external device. A suitable plug connector (P/N 2098690) for the *peripheral control input* connection is provided with the Installation Kit. See "User I/O Connections" on page 5-16 for specifications of the peripheral control input connection ports.

The *reset button* is also located on the power panel. When you press the reset button, the instrument software is reloaded from the data system. See "Resetting the System" on page 6-13 for information on resetting the mass spectrometer.

The USB port allows the internal computer to communicate with other devices of the GC/MS system. Do not connect any device to this port other than dedicated Thermo Fisher Scientific devices.

Power Column

The power column at the rear side of the instrument provides external connections for mains supply, gas, and Ethernet communication. See Figure 3-6.



Figure 3-6. Power column

Located at the top left side is the Ethernet port for connecting the mass spectrometer to the data system computer.

NOTICE For Q Exactive GC and Exactive GC GC/MS systems, a cable is provided to power the forepump from the topmost power outlet. ▲

The power connector for the mains supply is located below the two power outlets. Q Exactive GC and Exactive GC instruments are designed to operate at a nominal voltage of 230 V AC, 50/60 Hz. Line voltages can vary between a minimum of 207 V AC and a maximum of 253 V AC. Connect the power cord of the instrument to a wall receptacle that is fused with 15 A or 16 A. Above the gas ports, a ground bolt provides a protected earth connection for the ground wires of other devices of the GC/MS system.

The ports for nitrogen gas allow connecting a TeflonTM hose from the gas supply of the laboratory to the instrument and a supply of high-purity nitrogen gas for the C-Trap supply. (See also "Gas Supply" on page 3-30.) The required gas pressure is 800 ± 30 kPa (8 ± 0.3 bar, 116 ± 4 psi).

Vacuum System Controls

An interface for RS-485 data connects the TMPs to the vacuum control board. The vacuum gauges of the mass spectrometer are controlled by the same board. (See "Vacuum Control Board" on page 3-34.)

Vacuum Gauges

As shown in Table 3-4, vacuum in the mass spectrometer is measured in two regions.

|--|

| Region | Typical values | Gauge type | Name in Tune software |
|-------------------|----------------|-----------------|-----------------------|
| Quadrupole region | 3E-05 mbar | Cold Cathode | High Vacuum |
| Orbitrap analyzer | < 8E-10 mbar | Cold cathode | Ultra High Vacuum |

The vacuum is monitored by two vacuum gauges:

- The vacuum in the quadrupole region is monitored by a Compact Cold Cathode Gauge (IKR 251, manufacturer: Pfeiffer Vacuum).
- The vacuum in the Orbitrap analyzer chamber is monitored by a Compact Cold Gauge (IKR 270, manufacturer: Pfeiffer Vacuum).

Ion Optics of the Q Exactive GC Mass Spectrometer

Figure 3-7 shows the schematic view of the Q Exactive GC mass spectrometers. With the exception of the quadrupole, voltages for the elements of the ion optics are provided by the ion optic supply DC board (See page 3-33.) and the ion optics supply RF board. (See page 3-33.) The quadrupole voltages are supplied by a dedicated PCB. See page 3-33.



Figure 3-7. Schematic of the Q Exactive GC MS

Ion Optics of the Exactive GC Mass Spectrometer

Figure 3-8 shows the schematic view of the Exactive GC mass spectrometer. With the exception of the quadrupole, voltages for the elements of the ion optics are provided by the ion optic supply DC board (See page 3-33.) and the ion optics supply RF board. (See page 3-33.) The quadrupole voltages are supplied by a dedicated PCB. See page 3-33.



Figure 3-8. Schematic of the Exactive GC MS

Ion Source of the Q Exactive GC and Exactive GC Systems

There are three types of ion sources available for the Q Exactive GC and Exactive GC mass spectrometers: an electron ionization (EI) source, a chemical ionization (CI) source that enables that enables positive ion chemical ionization (PCI) and negative ion chemical ionization (NCI), and a combination EI/PCI/NCI source. All available ion sources include

an ion volume, repeller, source lenses, an RF lens, and dual filaments and are programmable from 50 °C to 350 °C. Figure 3-9 provides images of the three available ion volumes.





The ion source parts are contained in an ion source cartridge. See Figure 3-10.





The ion source cartridge is removable while the mass spectrometer is under vacuum. For removal instructions see "Removing the Ion Source Cartridge from the Q Exactive GC or Exactive GC System" on page 8-15. For cleaning instructions see "Cleaning the Q Exactive GC or Exactive GC Ion Source Cartridge and Durable Components" on page 8-38.

The *injection flatapole* is a square array of flat metal electrodes that acts as an ion focusing and as an ion pre-filtering device (Figure 3-11). An RF voltage that is applied to the electrodes (injection flatapole RF) gives rise to an electric field that focuses the ions along the axis of the lens. A DC offset voltage is applied to the injection flatapole (injection flatapole DC).



Figure 3-11. Injection flatapole

The *inter-flatapole lens* is a metal plate with a small hole through which the ion beam can pass. A DC potential is applied to the lens to aid in ion transmission. The lens also acts as a vacuum baffle between the source and analyzer ion optics chambers.

Analyzer Ion Optics of the Q Exactive GC and Exactive GC Mass Spectrometers

The *bent flatapole* always acts as an ion transmission device. It guides the ions through a 90° arc from the injection flatapole to the quadrupole and removes the neutral gas jet and passing through the injection flatapole. Because of the bent shape of the flatapole, the neutral particles cannot follow the bent path of the flatapole. The region around the bent flatapole is pumped by the interstage inlet IS1 of the source TMP.

An RF voltage is supplied through a separate RF vacuum feedthrough to the bent flatapole electrodes. A common mode DC offset voltage (bent flatapole DC) can be set. The combination of inner and outer *TK lens* (Turner-Kruger lens) focuses the ion beam into the quadrupole. It also shields the bent flatapole from the RF voltage applied to the quadrupole and vice versa. Additionally, the TK lens acts as vacuum baffle between bent flatapole and quadrupole. Furthermore, the lens assembly ensures the accurate and automatic alignment of bent flatapole and quadrupole. The quadrupole is described in the next topic. The quad exit lens focuses the ions coming from the quadrupole into the transfer multipole. The split lens is used to start and stop the injection of ions into the mass analyzer. It provides a high deflection voltage most of the time so that ions are deflected into a baffle except when they are to be allowed into the C-Trap. The fast switching of the ion beam ensures the precise determination of the ion injection time that is required for Automatic Gain Control (AGC). After passing the RF-only *transfer multipole*, which acts as another transmission device, the ions enter the C-Trap through its entrance lens.

Quadrupole Mass Filter

The *quadrupole* is a square array of precision-machined and precision-aligned hyperbolic-profile round rods. See Figure 3-12. Quartz spacers act as electrical insulators between adjacent rods.



Figure 3-12. Quadrupole

The quadrupole assembly is located in the source chamber between the TK lens and the transfer multipole. In addition to the quadrupole, the assembly includes the exit lens and the split lens.

In a quadrupole rod assembly, rods opposite each other in the array are connected electrically. Thus, the four rods can be considered as two pairs of two rods each. RF and DC voltages are applied to the rods and these voltages are ramped during the scan. Voltages of the same amplitude and sign are applied to the rods of each pair. However, the voltages applied to the different rod pairs are equal in amplitude but opposite in sign. See Figure 3-13.

The quadrupole board provides the voltages for operating the quadrupole. See page 3-33. The RF voltage applied to the quadrupole rods is of constant frequency (between 825–845 kHz) and varies from 0 to 6700 V peak-to-peak amplitude. The DC voltage varies from 0 to ± 500 V.



Figure 3-13. Polarity of the RF and DC voltages applied to the rods of the quadrupole mass filter

In Figure 3-14, the solid line represents the combined RF and DC voltage applied to one rod pair, and the dashed line represents the combined RF and DC voltage applied to the other rod pair. The RF-to-DC-voltage ratios and their values determine the range of mass-to-charge ratios to be transmitted through the quadrupole mass filter.



Figure 3-14. Magnitude of the RF and DC voltages applied between the rods of the quadrupole mass filter

In the mass spectrometer, the rods of the quadrupole are supplied with a variable ratio of RF voltage and DC voltage (Figure 3-14). For each injection, controlled by the split lens, the quad RF amplitude and DC voltage are set to fixed values. Under these conditions, only ions of a certain range of m/z ratios are maintained within bounded oscillations as their velocity carries them through the mass filter. At the same time, all other ions undergo unbounded oscillations. These ions strike one of the rod surfaces, become neutralized, and are pumped away, or they are ejected from the rod assembly.

The quadrupole offset voltage is a DC potential applied to the quadrupole rods in addition to the filtering DC voltage. The offset voltage applied to the two rod pairs of the assembly is equal in amplitude and equal in sign. The quadrupole offset voltage accelerates or decelerates ions and, therefore, sets the translational kinetic energy of the ions as they enter the quadrupole rod assembly.
Curved Linear Trap

On their way from the ion source to the Orbitrap analyzer, ions move through the gas-free RF transfer multipole into the gas-filled curved linear trap (C-Trap). See Figure 3-7 on page 3-14. Ions entering the C-Trap lose their kinetic energy in collisions with nitrogen bath gas and get collected near the middle part of the C-Trap. The nitrogen collision gas (bath gas) is used for dissipating the kinetic energy of injected ions and for cooling them down to the axis of the C-Trap.

Voltages on the end apertures of the C-Trap (entrance and exit apertures) are elevated to provide a potential well along its axis. These voltages may be later ramped up to squeeze ions into a shorter thread along this axis. The RF to the C-Trap (Main RF) as well as the entrance and exit DC voltages are provided by the C-Trap RF main board. (See page 3-35.) High voltages to the lens system are provided by the central electrode high-voltage power supply board. (See page 3-35.)

In the Q Exactive GC mass spectrometer, a *collector* is mounted behind the HCD collision cell. This collector is used for an independent C-Trap charge detection, which periodically (every 5–10 seconds) checks and adjusts the accuracy of the Automatic Gain Control. The collector is also used in some of the diagnostic procedures of the instrument.

In the Exactive GC mass spectrometer, a *collector* is mounted behind the C-Trap exit lens. This collector is used for an independent C-Trap charge detection, which periodically (every 5–10 seconds) checks and adjusts the accuracy of the Automatic Gain Control. The collector is also used in some of the diagnostic procedures of the instrument.

Orbitrap Analyzer

The heart of the Orbitrap[™] analyzer is an axially-symmetrical mass analyzer. It consists of a spindle-shape central electrode surrounded by a pair of bell-shaped outer electrodes. See Figure 3-15. The Orbitrap analyzer employs electric fields to capture and confine ions.



Figure 3-15. Schematic of Orbitrap cell and example of stable ion trajectory

Extraction of Ion Packets

For ion extraction, the RF on the rods of the C-Trap is ramped off and extracting voltage pulses are applied to the electrodes, pushing ions orthogonally to the curved axis through a slot in the inner electrode. Because of the initial curvature of the C-Trap and the subsequent lenses, the ion beam converges on the entrance into the Orbitrap analyzer. The lenses that follow the C-Trap (Z-lens) also act as differential pumping slots and cause spatial focusing of the ion beam into the entrance of the Orbitrap analyzer. Ions are electrostatically deflected away from the gas jet, thereby eliminating gas carryover into the Orbitrap analyzer.

Owing to the fast pulsing of ions from the C-Trap, ions of each mass-to-charge ratio arrive at the entrance of the Orbitrap analyzer as short packets that are only a few millimeters long. For each mass-to-charge population, this corresponds to a spread of flight times of only a few hundred nanoseconds for mass-to-charge ratios of a few hundred Daltons per charge. Such durations are considerably shorter than a half-period of axial ion oscillation in the C-Trap. When ions are injected into the Orbitrap analyzer at a position offset from its equator (See Figure 3-16.), these packets start coherent axial oscillations without the need for any additional excitation cycle.

The evolution of an ion packet during the increase of the electric field is shown schematically in Figure 3-16. When the injected ions approach the opposite electrode for the first time, the increased electric field (owing to the change of the voltage on the central electrode) contracts the radius of the ion cloud by a few percent. The applied voltages are

adjusted to prevent collision of the ions with the electrode. A further increase of the field continues to squeeze the trajectory closer to the axis, meanwhile allowing for newly arriving ions (normally, with higher m/z) to enter the C-Trap as well. After ions of all m/z have entered the Orbitrap analyzer and moved far enough from the outer electrodes, the voltage on the central electrode is kept constant and image current detection takes place.



Figure 3-16. Principle of electrodynamic squeezing of ions in the Orbitrap analyzer as the field strength is increased

NOTICE Q Exactive GC and Exactive GC instruments can fill the C-Trap in parallel to acquisition of the transient in the Orbitrap analyzer. ▲

Measuring Principle

In the mass analyzer shown in Figure 3-15 on page 3-22, stable ion trajectories combine rotation around an axial central electrode with harmonic oscillations along it. The frequency w of these harmonic oscillations along the z-axis depends only on the ion's mass-to-charge ratio m/z and the instrumental constant k:

$$\omega = \sqrt{\frac{z}{\overline{m}} \times k}$$

Two split halves of the outer electrode of the Orbitrap analyzer detect the image current produced by the oscillating ions. By Fast Fourier Transformation (FFT) of the amplified image current, the instrument obtains the frequencies of these axial oscillations and therefore the mass-to-charge ratios of the ions.

Ion Detection

During ion detection, the central electrode and the additional electrode, which deflects ions during injection and compensates electric field imperfections during the measurement (See Figure 3-16 on page 3-23.), are maintained at very stable voltages so that no mass drift can take place. The outer electrode is split in half at z=0, allowing the ion image current in the axial direction to be collected. The image current on each half of the outer electrode is differentially amplified and then undergoes analog-to-digital conversion before processing using the fast Fourier transform algorithm.



Figure 3-17. Approximate shape of ion packets of different *m/z* after stabilization of voltages

As mentioned above, stable ion trajectories within the Orbitrap analyzer combine axial oscillations along the z-axis with rotation around the central electrode and vibrations in the radial direction. (See Figure 3-15 on page 3-22.) For any given m/z, only the frequency of axial oscillations is completely independent of initial ion parameters, whereas rotational and radial frequencies exhibit strong dependence on initial radius and energy. Therefore, ions of the same mass-to-charge ratio continue to oscillate along z together, remaining in-phase for many thousands of oscillations.

In contrast to the axial oscillations, the frequencies of radial and rotational motion will vary for ions with slightly different initial parameters. This means that in the radial direction, ions dephase orders of magnitude faster than in the axial direction, and the process occurs in a period of only 50–100 oscillations. After this, the ion packet of a given m/z assumes the shape of a thin ring, with ions uniformly distributed along its circumference. See Figure 3-17. Because of this angular and radial smearing, radial and rotational frequencies cannot appear in the measured spectrum. Meanwhile, axial oscillations will persist, with axial thickness of the ion ring remaining small compared with the axial amplitude. Moving from one half outer electrode to the other, this ring will induce opposite currents on these halves, thus creating a signal to be detected by differential amplification.

HCD Cell

The HCD cell¹ consists of a straight multipole mounted inside a metal tube, which is connected in direct line-of-sight to the C-Trap. It is supplied with a collision gas to provide increased gas pressure inside the multipole. The C-Trap is directly attached to the HCD cell, so part of the collision gas flows into the C-Trap to serve as bath gas. See "Gas Supply" on page 3-30 for details. The ion optic supply DC board provides all RF and DC voltages necessary for operating the HCD cell. (See page 3-33.)

For HCD (Higher Energy Collisional Dissociation), ions are passed through the C-Trap into the HCD cell. The offset between the C-Trap and HCD is used to accelerate the precursor ions into the gas-filled cell. A potential gradient is applied to the HCD cell to provide fast extraction of ions, such that it returns ions at a reliable rate.

The spectra of fragments generated in the HCD cell and detected in the Orbitrap analyzer are comparable to the typical fragmentations patterns obtained on triple-quadrupole instruments. Refer to the QuickStart Guide for your instrument for more information.

¹ The Exactive GC does not contain an HCD cell.

Vacuum System

The vacuum manifold encloses the ion source interface, ion guides, C-Trap, and the Orbitrap analyzer. The vacuum manifold consists of thick-walled aluminum chambers with machined flanges on the front, sides, and bottom, and various electrical feedthroughs and gas inlets. The vacuum manifold is divided into three chambers. The region inside the first chamber is evacuated by a rotary-vane pump (forepump). The region inside the second chamber, called the source chamber, is evacuated by a turbomolecular pump (source TMP). The region inside the third chamber, called the analyzer chamber, is evacuated by another turbomolecular pump (analyzer TMP). Figure 3-18 shows a schematic overview of the vacuum system, Table 3-5 shows the vacuum regions of the mass spectrometer.



Figure 3-18. Schematic of vacuum system in Q Exactive GC and Exactive GC mass spectrometers

| T-LL- 9 F | 1/ | | |
|------------|--------|---------|----------|
| ladie 3-5. | vacuum | regions | overview |

| Region in instrument | Vacuum [mbar] | applied by |
|---|---------------------|------------------|
| EI/CI ion source Injection flatapole Bent flatapole | < 2E-5 ^ª | Source TMP IS1 |
| Transfer multipole Quadrupole | < 3.2E-05 | Source TMP HV |
| Z-lens | | Analyzer TMP IS2 |
| Region between Z-lens and Orbitrap analyzer | | Analyzer TMP IS1 |
| Orbitrap analyzer | < 6E-10 | Analyzer TMP HV |

^a Pressure will vary with helium carrier gas flow and CI reagent gas flow.

See page 3-13 for information about the vacuum gauges in the Q Exactive GC and Exactive GC mass spectrometer.

Turbomolecular Pumps

| | Two turbomolecular pumps (TMPs) provide the vacuum for the mass spectrometer. The TMPs are controlled by individual controllers and powered by +24 V DC (480 W) power supplies. Power for the TMPs is turned off by the main power circuit breaker switch, but not by the electronics service switch. The TMPs are air cooled by fans that are mounted in fan inserts on the bottom of the instrument. |
|--------------|---|
| | Pump controllers provide power to and control of the TMPs. The status of each TMP (such as temperature or rotational speed) is sent from the TMP controller to the vacuum control board. See page 3-34. |
| Analyzer TMP | |
| | The vacuum in the analyzer chamber is created by a second three-stage split flow TMP (TURBOVAC TW 290/20/20-UHV, manufacturer: Oerlikon Leybold Vacuum). The pump mounts onto the bottom of the vacuum manifold. The analyzer TMP has three pumping inlets (see Figure 3-18 on page 3-26): |
| | • A 20 L/s interstage inlet (IS2) in the molecular drag section of the pump, which evacuates the Z-lens region. |
| | • A 20 L/s interstage inlet (IS1) about half way down the rotor stack, which evacuates the region between Z-lens and Orbitrap analyzer. |
| | • A 250 L/s high-vacuum (HV) inlet at the top of the rotor stack, which evacuates the UHV (Orbitrap analyzer) chamber. |
| | The interstage inlet IS1 of the source TMP provides the forevacuum for the analyzer TMP. |
| | For a detailed description of the analyzer TMP and for instructions on user maintenance, refer to the handbook for the pump. See also "Maintenance of the Analyzer TMP" on page 8-10. |
| Vent Valve | |
| | The vent valve is a solenoid-operated valve that allows the vacuum manifold to be vented. The vent valve is closed when the solenoid is energized. The vacuum control board switches the vent valve. |
| | The vacuum manifold is vented when external power is removed from the instrument. (Power is removed from the instrument by a power failure or by placing the main power circuit breaker in the Off (O) position.) Power is provided to the vent valve for a short time after the external power is removed. If external power is not restored to the instrument within this time, power to the vent valve solenoid is shut off. When power to the vent valve solenoid is shut off, the vent valve opens |

Functional Description Vacuum System

and the manifold is vented with nitrogen. See Figure 3-18 on page 3-26 and Figure 3-19 on page 3-30. The vent valve closes after power is restored to the instrument.

System Bakeout

| | After the system has been open to the atmosphere (for example, during maintenance work or a power outage), the vacuum deteriorates due to contaminations of the inner parts of the vacuum system caused by moisture. These contaminations must be removed by heating the vacuum system by a system bakeout. See "Baking Out the System" on page 8-11 for instructions on performing a system bakeout. |
|-----------------|--|
| Bakeout Devices | |
| | To provide the high temperatures required for performing a system bakeout, the mass spectrometer is equipped with two halogen bulbs inside the vacuum chamber. Furthermore, two heating cartridges are built into the block that serves as housing for the analyzer TMP. |
| Bakeout Control | |
| | For a system bakeout, the instrument software simultaneously switches all heaters by relays. The vacuum control board controls the bakeout procedure. For example, the heaters are switched off in case of a failure of the fan below the analyzer TMP. |
| | NOTICE Individual printed circuit boards also have devices for checking the actual temperature. ▲ |
| Cooling Fans | |
| | Six fans provide cooling for Q Exactive GC and Exactive GC mass spectrometers. On the right instrument side, a fan insert with four fans cools the electronic boards. On the left instrument side, a second insert with two fans cools the analyzer chamber and the analyzer TMP. From the rear of the mass spectrometer, air is drawn in through fan filters. The exhaust air is expelled from the ventilation slots on the sides of the mass spectrometer. |
| | The vacuum control board monitors all fans within the instrument. During a system bakeout, it switches off one of the two fans below the analyzer TMP. In case of a fan failure, the board triggers an alert in the Tune software. In case of a failure of the fans below the analyzer TMP, no bakeout procedure is possible. |
| | NOTICE In addition to the fans described in this topic, various printed circuit boards are equipped with individual fans. ▲ |

Gas Supply

Q Exactive GC and Exactive GC mass spectrometers require ultra high-purity (>99.999%) nitrogen for the collision gas (bath gas) of the C-Trap and for the collision gas for the HCD cell¹. Nitrogen is also used to vent the vacuum manifold with the vent valve if the system is shut down. A nitrogen gas cylinder of a lesser purity may be used for venting the instrument. The required pressure is 800 ± 30 kPa (8 ± 0.3 bar, 116 ± 4 psi). The vented vacuum manifold is protected against overpressure by pressure relief valves and a glass manifold cover over the ion source. Figure 3-7 shows a schematic of the gas supply in the instrument.



Figure 3-19. Schematic of gas supply

NOTICE Calibration gas is composed of perfluorotributylamine vapor introduced with atmospheric air at very low flow. ▲

¹ The Exactive GC mass spectrometer does not have an HCD cell.

Gas Distribution Within the Instrument

Nitrogen from the gas supply in the laboratory enters the instrument through two separate connectors on the power column at the rear side of the instrument. See also Figure 3-6 on page 3-11.

The gas flow from the left nitrogen port is directed through TeflonTM tubing to the vent valve

The gas flow from the right nitrogen port is directed through brass tubing to a pressure regulator, which keeps the gas pressure to C-Trap and HCD cell¹ constant. From the regulator, the collision gas is led to the HCD cell next to the C-Trap (flow rate: ~0.5 mL/min). In the Q Exactive GC and Exactive GC mass spectrometers, an electronic pressure regulator sets the nitrogen pressure according to the operating mode of the instrument and the chosen user setting. The nitrogen gas leaking from the HCD cell is used for ion trapping and cooling in the C-Trap.

¹ The Exactive GC mass spectrometer does not have an HCD cell.

Printed Circuit Boards

| | Q Exactive GC and Exactive GC mass spectrometers are controlled by a PC running the Xcalibur [™] software suite. The software controls all aspects of the instrument. The main software elements are the control of ion detection and the control of the Orbitrap analyzer. The following pages contain a short overview of the various electronic boards of the mass spectrometer. |
|--------------|---|
| | The electronics of the mass spectrometer contains complicated and numerous circuits. Therefore, only qualified and skilled electronics engineers should perform servicing. |
| | A Thermo Fisher Scientific field service engineer should be called if servicing is required. It is further recommended to use Thermo Fisher Scientific spare parts only. Before calling a service engineer, try to localize the defect by means of errors indicated in the Tune software. A precise description of the defect will ease the repair and reduce the costs. |
| Preamplifier | |
| | The preamplifier board is a broadband amplifier with high-resistive differential inputs. It converts the image current, which is induced by the ions oscillating in the Orbitrap analyzer, to a proportional output voltage. The preamplifier interfaces through coaxial cables directly to the data acquisition board, which also provides the electric power for the preamplifier. After analog-to-digital conversion on the data acquisition board, the output voltage undergoes further Fourier transformation on the internal computer. |

Data Acquisition Board (DAQ Board)

The data acquisition (DAQ) board converts detected ion signals coming from the preamplifier to digital form. Then it sends the digital signals through a USB connection to the main board of the internal computer. The SPI bus is used for transmitting set commands and readbacks. A trigger input is used for synchronizing the DAQ board with the FT adapter board. By means of a relay, the DAQ board provides the electric power for the preamplifier.

Internal Computer (Data Acquisition Unit)

The internal computer controls the instrument's electronics and runs software that is downloaded from the data system computer. The internal computer performs the Fast Fourier Transformation (FFT) of the image current after it has been converted by the DAQ board.

| The internal computer communicates with the data system computer |
|--|
| through a 1 Gbit Ethernet switch. Internal USB connections connect it |
| to vacuum control board, data acquisition board, and FT adapter board. |
| An external USB port on the power panel (See Figure 3-5 on page 3-9.) |
| enables the internal computer to communicate with dedicated devices of |
| the GC/MS system. |

Source Board

In Q Exactive GC and Exactive GC systems, the source board controls the CI gas flow valves.

The source board distributes power to the ion gauges and the nitrogen gas valves—including the vent valve. Two connections to the I/O board allow the source board to communicate with other devices of the GC/MS system.

The system status LEDs on the front side of the instrument (See Figure 3-3 on page 3-7.) are controlled by the source board. The displayed status information partially comes from other boards. The board communicates through the SPI bus.

Ion Optic Supply DC Board

With the exception of the quadrupole, the ion optic supply DC board provides the DC voltages for all ion-optical components in front of the C-Trap as well as the HCD voltages¹. The ion optic supply DC board, however, does not provide voltages for the EI/CI ion source

Ion Optic Supply RF Board

With the exception of the quadrupole, the ion optic supply RF board provides the RF voltages for all ion-optical components in front of the C-Trap as well as the HCD voltages. It has an RF detector for the RF output control. Furthermore, the board provides the DC voltages for the split lens and the injection flatapole.

Quadrupole Board

The quadrupole board (quad board) supplies RF voltages and DC voltages for the quadrupole. See "Quadrupole Mass Filter" on page 3-18. Set values and readbacks of voltages, currents, and temperatures are communicated through the SPI bus.

¹ Exactive GC systems do not have HCD cells.

FT Adapter Board

| The FT adapter board links the internal computer to the various system components. Its main function is the control of scan events within the instrument. The board contains a micro controller, an FPGA (Field Programmable Gate Array), and serial port connectors. |
|--|
| Through the USB interface, the internal computer transmits set commands for system components to the FT adapter board. By the same interface, the internal computer requests readback values. The FT adapter board converts the set commands during the scan and sends the readback data through USB to the internal computer. The master interface of the Extended Orbitrap SPI bus of the FT adapter board serves for transmitting the set commands and readbacks. |
| |
| Various boards communicate system parameters and monitor readbacks over the Serial Peripheral Interface (SPI) bus. The master interface of the SPI bus is located on the FT adapter board. |
| |
| The vacuum control board controls the vacuum system. Depending on the quality of the vacuum and the status of the TMPs, it switches the vacuum gauges, the pumps, and the 230 V relays. When the vacuum measured by the Ion Gauge 2 is better than 1E-8 mbar, the vacuum control board switches on the power supply of the high voltage electronics. |
| On the vacuum control board, analog signals from vacuum gauges are converted to digital signals and passed to the internal computer through a USB connection. TMPs are attached to a serial port connector and this is connected by the signal lines to the vacuum control board. (See "Vacuum System" on page 3-26.) |
| The board controls external relays with 24 V DC connections. In addition to the vent valve, the board also switches the valve that controls the flow of the HCD collision gas. The vacuum control board controls the bakeout heaters. It also monitors six fans within the instrument; it switches off the two fans below the analyzer TMP during a system bakeout. In case of a fan failure, the board triggers an alert in the Tune software. |
| |

C-Trap RF Board

The C-Trap RF board operates the C-Trap with four phases of RF voltage (Main RF) and three pulsed DC voltages (PUSH, PULL, and OFFSET). It allows simultaneous switching off the RF and pulsing of each C-Trap electrode. See "Orbitrap Analyzer" on page 3-22 for further information. The board also provides the entrance voltage and the exit voltage to the C-Trap. The board communicates with the other boards through the SPI bus.

CE HV Supply Board

The central electrode high-voltage supply board provides five voltages for the ion optics of Q Exactive GC and Exactive GC mass spectrometers:

- Two high voltages supply lenses that follow the C-Trap.
- Two DC voltages and one AC voltage are applied to the RF C-Trap main board to be used as focusing potentials for the C-Trap.

Furthermore, the board supplies six DC voltages to the Orbitrap analyzer:

- Four central electrode (CE) voltages: CE POS, CE NEG, CE LOW+, and CE LOW-
- Two deflector electrode (DE) voltages: DE HIGH and DE LOW

For positive ions, the CE voltages are negative and the DE voltages are positive. The maximum CE voltage is 5 kV and the maximum DE voltage is 1.25 kV. See "Orbitrap Analyzer" on page 3-22 for further information.

Also, the analog-to-digital (AD) conversion of the PT-100 signal takes place on this board.

The board communicates through the SPI bus. A Peltier element on the rear side of the board serves as means of heat dissipation.

CE Pulser Board

The central electrode pulser board switches the injection and measurement voltages for the central electrode and the deflector electrode of the Orbitrap analyzer. Resistor-capacitor circuits on the board convert the switching pulse into a smooth transition between the voltages. Furthermore, the board switches the polarity of the central Orbitrap electrode. The temperature of the Orbitrap analyzer is measured by the PT-100 temperature probe. The signal of the probe is converted and analyzed on the CE pulser board. Then it is sent to the CE HV supply board where analog-to-digital conversion takes place.

Power Supply DAQ Board

The power supply DAQ board provides the voltages that are required by the data acquisition board. The board is equipped with a fan for heat dissipation.

I/O Board

The input/output (I/O) board provides the interfaces for data exchange between the mass spectrometer and other devices of the GC/MS system. It contains a reset switch, four relay outputs and a digital inlet port. (See "Peripheral Control" on page 3-9.) It is connected to the FT adapter board and to the source board.

Chapter 4 Safety

This chapter provides information about machine safety.

Contents

- "Safety Symbols and Signal Words in This Manual" on page 4-2
- "Safety Symbols on the Instrument" on page 4-3
- "Intended Use" on page 4-5
- "Electric Safety Precautions" on page 4-7
- "In Case of Emergency" on page 4-8
- "Residual Hazards" on page 4-10

Safety Symbols and Signal Words in This Manual

Notices concerning the safety of the personnel operating the Q Exactive GC or Exactive GC mass spectrometer appear different from the main flow of text. Safety notices include the following:

Always be aware of what to do with, and the effect of, safety information.
 CAUTION Points out a hazardous situation that can lead to minor or medium injury if not avoided.
 WARNING Points out a hazardous situation that can lead to severe injury or death if not avoided.
 DANGER Points out a hazardous situation that will lead to severe injury or death if not avoided.

Observing This Manual

This manual must always be kept near the instrument to be available for quick reference.



Be sure to read and comply with all precautions described in this manual.

System configurations and specifications in this manual supersede all previous information received by the purchaser.

Safety Symbols on the Instrument

Table 4-1 lists all safety labels on the instrument and their respective positions. See the indicated safety notices to prevent risk of harm to the operator and to protect the instrument against damage. If present, read and follow the instructions on the labels.

Table 4-1.Safety labels on the instrument

| Label | Label description | Label position |
|-------|---|---|
| | Four labels of this type are attached to the power panel on the left side of the instrument. See red circles in figure. The label indicates the presence of electric current at the switches or contact ports. | Unit Operating Mode Control Contro Control Control Control |
| | This label is attached to the right panel on the rear side of the instrument. The label indicates the presence of electric current and moving parts inside the instrument. See page 5-12 for details. | <u>A</u> •1 |



This label is attached to the power column at the rear side of the instrument, below the power outlets. See white circle in figure.

The label indicates the presence of electric current at the ports at the power column. See page 5-8 for details.



Rating Plate

To correctly identify the instrument when communicating with Thermo Fisher Scientific, always have the information from the rating plate available. The rating plate is attached to the power column at the rear side of the instrument. See Figure 4-1.

| | SCIENTIFIC Hanna-Kunath-Str. 11, 28199 Bremen, Germany |
|--|--|
| | FREQUENCY RANGE AC VOLTAGE 1~ CURRENT MAX 1~ year of manufacture 2012 Made in Germany |
| | SERVICE BY QUALIFIED PERSONNEL ONLY |
| Ethernet Forepump | Mass Spectrometer MODEL: EXACTIVE PLUS SERIAL No: SN02007P |
| 1000 Base 7 On/Off Thermo Fisher | |
| EXACTIVE SCIENTIFIC | |
| This product is manufactured under, and covered by, one or more of the following U.S. patents: 5157260 5245186 553897 5572023 5581090 | |
| 9060740 9709990 5060546 007703 6249999 6528784 6687474 697239 6872940 6967261 6998609 7009176 7053368 7145138 7199364 Re35413 7245669 7498571 7576318 7657387 7675031 7847243 | |
| This device compiles with part 15 of the FCC Rules. Operation is subject to the following two conditions: | |
| This device may not cause harmful interference, and This device must accept any interference received, including interference that may cause undesired operation. | |
| ThermoFisher SCIENTIFIC Harra-Kunath-Bir. 11, 28199 Braman, Garmany | |
| FREQUENCY RANGE 50-60Hz AC VOLTAGE ~ 230V 4/-10% CURRENT MAX ~ 15A yeer of menufacture 2012 Germany | |
| SERVICE BY QUALIFIED PERSONNEL ONLY Mass Spectrometer MODEL: EXACTIVE PLUS SERIAL No: SN02007P | |

Figure 4-1. Rating plate

Intended Use

Q Exactive GC and Exactive GC mass spectrometers are stand-alone Orbitrap[™] instruments with an ExtractaBrite[™] removable ion source for gas chromatography (GC) mass spectrometry (MS) high-throughput applications.



- The instrument is designed to be placed on a bench in the laboratory. It is not designed for use outdoors.
- The bench must be rated to support the weight of the instrument as outlined in the *Q Exactive GC and Exactive GC Preinstallation Requirements Guide*.
- The instrument is designed to be used exclusively with the TRACE 1310 GC and probes produced by Thermo Fisher Scientific.
- The instrument is designed for laboratory research use only. It is not designed for use in diagnostic or medical therapeutic procedures.

If the Q Exactive GC or Exactive GC mass spectrometer is used in a manner not specified by Thermo Fisher Scientific, the protection provided by the instrument could be impaired. Thermo Fisher Scientific assumes no responsibility and will not be liable for instrument damage and/or operator injury that might result from using the instrument with other GC systems and probes.

Notice on the Susceptibility to Electromagnetic Transmissions

Your instrument is designed to work in a controlled electromagnetic environment. Do not use radio frequency transmitters, such as mobile phones, in close proximity to the instrument.

Qualification of the Personnel

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Only employees of Thermo Fisher Scientific or personnel acting on behalf of Thermo Fisher Scientific are allowed to install Q Exactive GC and Exactive GC mass spectrometers.

Personnel that install or operate Q Exactive GC and Exactive GC mass spectrometers must have the following qualifications:

• Electrical Connections

The electrical installation must be carried out by qualified and skilled personnel (electrician) according to the appropriate regulations (for example, cable cross-sections, fuses, grounding connection). Refer to the *Q Exactive and Exactive GC Preinstallation Requirements Guide* for the specifications.

• General Operation

Q Exactive GC and Exactive GC mass spectrometers are designed to be operated by qualified laboratory personnel. Before starting, all users must be instructed about the hazards presented by the instrument and the used chemicals. The users must be advised to read the relevant Material Safety Data Sheets (MSDSs).

Permitted Materials

Q Exactive GC and Exactive GC mass spectrometers are designed to be operated with the following materials:

- Nitrogen gas: Used for the C-Trap bath gas and HCD¹ collision gas
- Forepump oil: Used for cooling, lubrication, and sealing of the forepump
- Optional reagent gases including: methane, isobutane, and ammonia.

NOTICE Use only the forepump oil indicated on the name plate and pump. In case other oils are used, the manufacturer (Oerlikon Leybold Vacuum) rejects all responsibility should any trouble occur. ▲

¹ Q Exactive GC systems only

Electric Safety Precautions

A WARNING

High Voltage. High voltages (up to 8 kV) capable of causing an electric shock are used in the instrument.

Observe the following safety precautions when you operate or perform service on your instrument:

- The instrument is properly grounded in accordance with regulations when shipped. You do not need to make any changes to the electrical connections or to the instrument's chassis to ensure safe operation.
- There are no customer serviceable parts inside. Never remove any housing or protective cover except were elsewhere permitted in this manual. When leaving the system, make sure that all protective covers and doors are properly connected and closed, and that heated areas are separated and marked to protect unqualified personnel.
- Do not turn on the instrument if you suspect that it has incurred any kind of electrical damage. Instead, disconnect the power cords of the mass spectrometer and contact a Thermo Fisher Scientific field service engineer for a product evaluation. Do not attempt to use the instrument until it has been evaluated. Electrical damage may have occurred if the system shows visible signs of damage, or has been transported under severe stress.
- Do not place any objects on top of the instrument—especially not containers with liquids—unless it is requested by the user documentation. Leaking liquids might get into contact with electronic components and cause a short circuit.

In Case of Emergency

- * To shut down the system in case of emergency
- Disconnect the power cord of the mass spectrometer to ensure that the instrument is free from all electric current. All power to the mass spectrometer, including the internal vacuum pumps, is shut off.

NOTICE Placing the main power circuit breaker switch (labeled Mainpower) on the power panel (Figure 4-2) in the Off (O) position may not be sufficient. ▲

A WARNING

Electric Current. Electric shock hazard. Do not use the electronics service switch to shut down the instrument. The electric components of the vacuum system will still be connected to the electric power supply and the pumps will remain running.



Main Power Circuit Breaker Switch

Figure 4-2. Power panel, showing main power circuit breaker switch and reset button



Figure 4-3. Rear side view of instrument

- 1. The Q Exactive GC and Exactive GC GC/MS forepump has an on/off switch that should remain in the on position so that the power to the GC/MS forepump can be maintained by the 230V power output of the MS.
- 2. Turn off the computer with its On/Off switch.
- **A WARNING Electric Current.** Electric shock hazard. Capacitors inside the instrument might still be charged even if the instrument is turned off. Wait for sufficient time before you remove the instrument housing.

Residual Hazards

Users of Q Exactive GC and Exactive GC mass spectrometers must pay attention to the following residual hazards.

- **WARNING Hazardous Chemicals.** The effluent of the forepump might contain noxious chemicals. The forepump eventually exhausts much of what is introduced into the mass spectrometer, including the small amount of oil vapor that mechanical pumps can emit. The connection of the forepump to an adequate exhaust system is mandatory!
- ▲ WARNING Suffocation Hazard. Accumulation of nitrogen gas could displace sufficient oxygen to suffocate personnel in the laboratory. Ensure that the laboratory is well ventilated. Local regulations may require a risk assessment for the workplace.
- **A** CAUTION Hazardous Chemicals. Samples and solvents might contain toxic, carcinogenic, mutagenic, or corrosive/irritant chemicals. Avoid exposure to potentially harmful materials. Always wear protective clothing, gloves, and safety glasses when you handle solvents or samples. Also contain waste streams and use proper ventilation. Refer to your supplier's Material Safety Data Sheet (MSDS) for proper handling of a particular compound.
- ▲ CAUTION Hot Surface. Touching parts of the forepump might cause burns. The forepump in function is hot and some surfaces could reach a temperature higher than 70 °C (158 °F). Switch off the pump and let it cool down before any intervention or take appropriate precautions. Always wear heat protective gloves when working on a pump that is "still warm from operation".
- ▲ CAUTION Hot Surface. Touching hot parts of the ion source interface might cause severe burns. During operation of the mass spectrometer, the ExtractaBrite removable ion source might reach temperatures of up to 350 °C, while the GC column transfer line might reach temperatures of up to 400 °C. To let the ion source interface cool down, set the ion source and transfer line temperatures to 25 °C. Wait until the ion source has cooled down to room temperature (for approximately 60 minutes) before you begin working on it. Do not leave the instrument unattended when the covers and front door are removed, exposing the hot source parts. Hot ion source parts might ignite combustible material. Keep combustible materials away from the ion source mount.

Personal Protective Equipment

This manual can only give general suggestions for personal protective equipment (PPE), which protects the wearer from hazardous substances. Refer to the Material Safety Data Sheets (MSDSs) of the chemicals handled in your laboratory for advice on specific hazards or additional equipment.

Eye Protection

The type of eye protection required depends on the hazard. For most situations, safety glasses with side shields are adequate. Where there is a risk of splashing chemicals, goggles are required.

Protective Clothing

When the possibility of chemical contamination exists, protective clothing that resists physical and chemical hazards should be worn over street clothes. Lab coats are appropriate for minor chemical splashes and solids contamination, while plastic or rubber aprons are best for protection from corrosive or irritating liquids.

Gloves

For handling chemical compounds and organic solvents, Thermo Fisher Scientific recommends the following gloves: white nitrile clean room gloves (Fisher Scientific P/N 19-120-2947B [size medium] or P/N 19-120-2947C [size large]; Thermo Scientific P/N 23827-0008 [size medium] or P/N 23827-0009 [size large]).

For handling hot objects, gloves made of heat-resistant materials (for example, leather) should be available.

Chapter 5 Installation

This chapter describes the conditions for an operating environment that will ensure continued high performance of your Q Exactive GC or Exactive GC system.

Contents

- "Safety Guidelines for Installation" on page 5-2
- "Placing the Instrument" on page 5-3
- "Laboratory Conditions" on page 5-8
- "Connecting the Instrument to the Gas Supply" on page 5-11
- "Setting Up Instrument Hardware and Adjusting System Parameters" on page 5-15

To be sure that your laboratory is ready for the installation of the Exactive Series system, you have to meet all requirements specified in the *Q Exactive GC and Exactive GC Preinstallation Requirements Guide*. This guide also provides comprehensive information to assist in planning and preparing your lab site. A printed version of the *Q Exactive GC and Exactive GC Preinstallation Requirements Guide* is part of the Preinstallation Kit. This kit is sent to your laboratory before the arrival of the Q Exactive GC or Exactive GC mass spectrometer.

Safety Guidelines for Installation

When installing the Q Exactive GC or Exactive GC system, pay attention to the following general safety guidelines.

- **WARNING** Suffocation Hazard. Accumulation of nitrogen gas could displace sufficient oxygen to suffocate personnel in the laboratory. Ensure that the laboratory is well ventilated. Local regulations may require a risk assessment for the workplace.
- **WARNING Hazardous Chemicals.** The effluent of the forepump might contain noxious chemicals. The forepump eventually exhausts much of what is introduced into the mass spectrometer, including the small amount of oil vapor that mechanical pumps can emit. The connection of the forepump to an adequate exhaust system is mandatory!
- **A** CAUTION Hazardous Chemicals. Samples and solvents might contain toxic, carcinogenic, mutagenic, or corrosive/irritant chemicals. Avoid exposure to potentially harmful materials. Always wear protective clothing, gloves, and safety glasses when you handle solvents or samples. Also contain waste streams and use proper ventilation. Refer to your supplier's Material Safety Data Sheet (MSDS) for proper handling of a particular compound.

Placing the Instrument

This section provides information that helps you positioning the instrument in the laboratory.

Instrument Dimensions

Q Exactive GC and Exactive GC systems always includes the TRACE 1310 GC and have maximum dimensions of h 95 cm (37 in.), w 91 cm (36 in.), l 148 cm (58 in.). Figure 5-1 shows a schematic view of the instrument with important instrument dimensions.

Additional clearance should be maintained above and to the right of the GC for samplers. The AS 1310 autosampler requires an additional 22 cm to the right of the GC. The TriPlus RSH autosampler requires and additional 32 cm to the right of the GC.





Workbench for Instrument

| | The workbench for the Q Exactive GC and Exactive GC systems must be capable of supporting approximately 250-280 kg, which includes the weight of the mass spectrometer plus the weight of the GC and any options such as an autosampler. The workbench surface must remain in a secure and level position when loaded. |
|-------------------|---|
| A CAUTION | Only workbenches with at least four legs provide sufficient stability for the Q Exactive GC and Exactive GC mass spectrometers. The workbench top must be dry and clean (free of grease). Thermo Fisher Scientific recommends using a workbench with a skidproof top. |
| Minimum Clearance | |
| | Allow at least 15 cm (6 in.) of clear space behind the system for proper air circulation and for clearance of the gas lines and electrical connections. This also provides sufficient space for accessing the fan filters on the rear side of the mass spectrometer. In addition, allow at least 92 cm (36 in.) of vertical clearance between the top of the mass spectrometer and any shelves above it. |
| | To allow shutting off the mass spectrometer in an emergency, free access to the power panel on the left side and to the power column on the rear side of the instrument must be possible at any time. |
| | NOTICE Avoid blocking the ventilation slots at the rear side of the mass spectrometer. Items might fall behind the instrument, inhibit airflow, and cause the system to overheat. Depending on the circumstances, either the Tune software will switch off the instrument and display an error message or the turbomolecular pump control will shut down the instrument and vent it. ▲ |

Moving the Instrument



NOTICE Before moving the instrument from one place to another, all participating personnel must carefully read and follow the instructions given in this manual. ▲

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Q Exactive GC and Exactive GC instruments are provided with four retractable handles. Each instrument is shipped on a pallet with the handles pulled out and fixed on the pallet. See Figure 5-2. Safety catches prevent the handles from unintentionally being retracted after they have been pulled out. Inspect the handles to verify that their safety catches are engaged before you start lifting the instrument. Push down the safety catch on a handle to slide it into the instrument.



Figure 5-2. Handles, fixed on the transport pallet

▲ CAUTION Heavy Load. Because of its weight of about 220 kg, handling the instrument alone might cause muscle strain and back injury. Lifting and moving the instrument requires the effort of at least *six persons* to keep the individual load within acceptable limits (maximum 40 kg for men or 15 kg for women for a duration of 5 seconds). The carriers must be trained in how to carry loads properly (for example, by rising from the knees with a straight back). Thermo Fisher Scientific recommends using a pallet jack to lift the mass spectrometer to the height of the workbench.

A CAUTION Heavy Objects. Mass spectrometer and forepump might move uncontrollably and cause injuries. Wear steel-reinforced safety shoes and gloves during installation or maintenance.

The instrument is shipped with two lifting devices, each providing sufficient space for three persons that are standing side by side. An instrument with attached lifting devices does not fit through a door with a width of 80 cm (32 in.), in contrast to the unpacked instrument alone. Furthermore, the six persons that carry the instrument require considerable space for maneuvering. Therefore, Thermo Fisher Scientific recommends using a pallet jack when moving the instrument into another room.

The following instructions assume that the instrument has been moved to the installation site with a pallet jack and the top cover of the transport crate has been removed.

* To move the instrument onto the workbench

- 1. Gather six persons and appoint one person that takes command and gives instructions to the remaining people.
- 2. Lift the instrument to the height of the working bench by using the pallet jack.
- 3. Remove the four clamps that fix the instrument to the transport pallet. See Figure 5-2.

- 4. Each lifting device consists of a folded metal sheet with holes and a twice bent tube. It comes with four hexagon screws, four washers, and two clamps. Mount each device onto the handles at one instrument side:
 - a. Place a clamp (pos. 2 in Figure 5-3) below each handle.



Labeled Components: 1=Lifting device; 2=clamp; 3=hexagonal screw; 4=washer

Figure 5-3. Lifting device

- b. Two diamond-shaped holes in the metal sheet of the lifting device indicate the place where the handles of the instrument shall be mounted to the device. Hold the device so that the yellow label on the lifting device is visible, which advises users to read the manual. Place the device on top of the handles, with the two ends of the twice bent tube pointing toward the instrument.
- c. Insert two screws (pos. 3 in Figure 5-3) with washers (pos. 4) at each side of a diamond-shaped hole and fasten the clamp with them. Repeat this for the other diamond-shaped hole. Make sure that the device is aligned parallel to the side of the instrument, and not twisted. Check that the lifting device is tightly attached to the handles.
- d. At the opposite side of the instrument, repeat the above steps with the other lifting device. The figure on the right shows a closeup view of a handle that is mounted to the lifting device. Note the diamond-shaped hole between the hexagonal screws.



The ends of the lifting devices must be aligned flush with each other as shown in Figure 5-4. Red circles in the figure indicate the positions of the diamond-shaped holes in the lifting devices.



Figure 5-4. Lifting devices attached to instrument (top view)

▲ CAUTION Top Heavy Load. The mass spectrometer might tip over while being moved in the laboratory and cause bodily injury or instrument damage. The instrument's center of gravity is at the top of the front side: the instrument has a tendency to tilt forward. When lifting the instrument, support the top of the instrument and keep the tilt angle below 5°; never exceed 10°.

- 5. On command, all six carriers lift off the instrument simultaneously—to prevent them from experiencing an uneven load distribution. Using the lifting devices, place the instrument onto the bench.
- 6. Remove the lifting devices from the handles.
- 7. The rear pair of the four support points for the instrument consists of wheels. Thus, only two persons are necessary for moving the instrument into its final position on a bench, while holding the two front handles. See Figure 5-2 on page 5-5 for information about the position of the support points.

* To store away the handles

Push down the spring (safety catch) of the handle by using a screw driver and shove the handle into its housing.

Laboratory Conditions

This section gives an overview of important requirements for the laboratory where the Q Exactive GC or Exactive GC mass spectrometer is placed. For details, refer to the *Q Exactive GC and Exactive GC Preinstallation Requirements Guide*.

Power and Gas Supply

The Q Exactive GC or Exactive GC mass spectrometer requires a dedicated wall outlets providing a nominal voltage of 230 V AC, 50/60 Hz, single phase. The forepump receives its power from the MS. A dedicated wall outlet is required for the GC and is required to be the same nominal voltage and phase as the mass spectrometer.

The components of the data system (computer, monitor, and Ethernet switch) require wall outlets at a nominal voltage of 230 V AC or 120 V AC, 50/60 Hz.





WARNING Electric Current. Electric shock hazard. Wrong usage of these ports might endanger personnel. Read and understand the Operating Manual to prevent risk of harm to the operator and to protect equipment against damage. To ensure that the instrument is free from all electric current, always disconnect the power cords of *mass spectrometer and forepump* before attempting any type of maintenance.
NOTICE Do not connect other gases than nitrogen to the nitrogen inlets of the mass spectrometer! This might affect instrument performance. The maximum pressure for the gas inlet is 830 kPa (8.3 bar, 120 psi). ▲

Laboratory Temperature

The mass spectrometer is designed to operate at a laboratory room temperature between 15 and 26 $^{\circ}$ C (59 and 78 $^{\circ}$ F).

NOTICE Do not put the mass spectrometer under an air duct, near windows, or near heating and cooling sources. Temperature fluctuations of 1 °C or more over a 10 minutes period can affect instrument performance. ▲

Humidity

The relative humidity of the operating environment must be between 40 and 70%, with no condensation. It is recommended that your laboratory be equipped with a temperature/humidity monitor to ensure that your laboratory is always within the required temperature and humidity specifications.

NOTICE Operating the mass spectrometer at very low humidity might cause the accumulation and discharge of static electricity, which can shorten the life of electronic components. Operating the mass spectrometer at high humidity might cause condensation, oxidation, and short circuits, and will also block the filters on the cooling fans. ▲

NOTICE A significant change of the humidity in the laboratory can affect the mass accuracy. If the humidity in the laboratory has changed significantly since the last mass calibration, Thermo Fisher Scientific recommends refreshing the mass calibration. \blacktriangle

Ventilation and Fume Exhaust

Consider the following safety guidelines for ventilation and exhaust.

A WARNING Suffocation Hazard. Accumulation of nitrogen gas could displace sufficient oxygen to suffocate personnel in the laboratory. Ensure that the laboratory is well ventilated. Local regulations may require a risk assessment for the workplace.

Vibration

Floors must be free of vibration caused, for example, by equipment in adjoining locations.

NOTICE Because of the natural vibration of the forepump during operation, it must not have any mechanical contact to the mass spectrometer with the exception of the vacuum hose. Otherwise, the vibration might affect instrument performance. Therefore, install the pump on the floor beneath the mass spectrometer and not near the system on the workbench. \blacktriangle

Airborne Noise Emission

The A-weighted emission sound pressure level created by the Q Exactive GC or Exactive GC mass spectrometer at work stations does not exceed 70 dB(A).

Connecting the Instrument to the Gas Supply

NOTICE Do not connect other gases than nitrogen to the nitrogen inlets of the Q Exactive GC or Exactive GC mass spectrometer! This might affect instrument performance. The maximum pressure for the gas inlet is 830 kPa (8.3 bar, 120 psi). ▲

* To connect the nitrogen source to the mass spectrometer

- Connect an appropriate length of Teflon[™] tubing to the nitrogen source in the laboratory. The Installation Kit contains 10 m (33 ft) of suitable Teflon tubing (OD 6 mm, see Chapter 9: "Replaceable Parts"). The connection for the Teflon hose to the nitrogen gas supply is not provided in the kit; you have to supply this part.
- 2. Connect the brass tubing supplied in the installation kit to the left nitrogen port that supplies the C-Trap and HCD gas. For optimal performance, and to protect against interruption by any air admitted into the nitrogen gas when a shared dewar or laboratory gas supply is changed, use a dedicated ultra high purity nitrogen cylinder to directly supply the C-Trap and HCD gas. The gas usage is less than 10 atm-mL/min in normal operation, so a compressed gas cylinder will last a long time. Attach the shared laboratory gas supply to the vent inlet, which has much higher usage, but only when the system is powered off and venting/purging. See the *Q Exactive and Exactive GC Preinstallation Requirements Guide* for additional information.

NOTICE If air is not properly purged from gas supply lines, the instrument leak check will report an oxygen leak until the air is removed. ▲



Figure 5-6. Connecting the gas supply

- ▲ WARNING Moving Parts and High Voltage. Risk of injury or electric shock. The interior of the instrument contains parts that are moving or that are at high voltages. When opening the instrument housing is necessary, call a Thermo Fisher Scientific field service engineer.
- **WARNING** Suffocation Hazard. Accumulation of nitrogen gas could displace sufficient oxygen to suffocate personnel in the laboratory. Ensure that the laboratory is well ventilated. Local regulations may require a risk assessment for the workplace.

Connecting the Q Exactive GC CI Gas Supply

If you are using chemical ionization on the Q Exactive GC or Exactive GC mass spectrometer, follow the steps below to connect the CI gas supply to the mass spectrometer.

1. Power off the Q Exactive GC or Exactive GC mass spectrometer and the TRACE 1310 GC. See "Shutting Down the System" on page 6-7 for instruction to shut down the mass spectrometer. Refer to the TRACE 1310 user documentation for instructions to shut down the GC.

2. Remove the screws on the front cover as shown below.





3. Attach the CI reagent gas to either port A or port B.



Figure 5-8. Connecting the CI gas supply

A CAUTION

Hazardous Chemicals. Some CI gases, such as ammonia, are toxic. Make sure that supply tubing and fittings are rated for the gas being plumbed. Make sure these gases are properly exhausted and all gas fittings on the system are leak-free. Check for leaks by pressurizing the gas lines, shutting off the gas supply, and ensuring that the pressure does not drop. If you have an electronic leak detector available, use it to detect leaks as well. Consult your local Environmental and Safety Regulations for information about how to properly exhaust fumes from your laboratory. Use stainless steel tubing, which is not supplied with the system, for corrosive gases.

A WARNING

Fire Hazard. Some CI gases, such as methane and isobutane, are flammable. Make sure these gases are properly exhausted and all gas fittings on the system are leak-free. Check for leaks by pressurizing the gas lines, shutting off the gas supply, and ensuring that the pressure does not drop. If you have an electronic leak detector available, use it to detect leaks as well. Consult your local Environmental and Safety Regulations for information about how to properly exhaust fumes from your laboratory.

Setting Up Instrument Hardware and Adjusting System Parameters

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Only employees of Thermo Fisher Scientific or personnel acting on behalf of Thermo Fisher Scientific are allowed to install the Q Exactive GC and Exactive GC mass spectrometers.

The Q Exactive GC and Exactive GC mass spectrometer and other devices shipped with it are installed by a Thermo Fisher Scientific field service engineer. During the installation, the service engineer will demonstrate the basics of equipment operation and routine maintenance.

When you want to connect the mass spectrometer to other equipment, refer to the manuals that came with the additional equipment.

The QuickStart Guide for your instrument gives an introduction on setting up and using the Q Exactive GC or Exactive GC mass spectrometer. For detailed information about changing the instrument parameters and developing experiments for the instrument, refer to the Software Manual or the Tune Help.

User I/O Connections

This section describes the specifications for the peripheral control connections. It contains the following topics:

- "Output Specifications" on page 5-16
- "Input Specifications" on page 5-17

Location and function of the peripheral control connections are described in "Peripheral Control" on page 3-9.

Output Specifications

The Q Exactive GC and Exactive GC mass spectrometer outputs correspond to the status functions listed below. The outputs are potential-free relay contacts, which are closed when the status indicated by the name is true.

The following outputs are available:

- Ready Out (Pins 1 and 2)
- Start Out (Pins 3 and 4)
- Valve 1 (Pins 5 and 6)
- Valve 2 (Pins 7 and 8)

Location and function of the peripheral control outputs are described on page 3-9. Figure 5-9 shows the circuit diagram and Table 5-1 lists the specifications of the peripheral control output.





| Tabla | Б1 | Output | oirouit | appoifications |
|-------|-----------|--------|---------|----------------|
| Idule | J-1. | υυιρυι | CIICUIL | specifications |

| Contact closed | $R_{on} < 0.2 \Omega$ |
|----------------|-------------------------|
| Contact open | $R_{off} > 1 \ G\Omega$ |
| Current | $I_{max} = 0.5 A$ |
| Voltage | $V_{max} = 30 V$ |
| Power | $P_{max} = 10 W$ |

Input Specifications

The Q Exactive GC and Exactive GC mass spectrometer provides one digital input to connect external devices.

The following input is available:

• Start In port (Pins 1 and 2)

Start In Input Specification

The Start In input is an input with internal pull-up resistor for connecting external relays contacts or open collector transistors. Start is triggered with the falling edge of input voltage.

Location and function of the Start In input are described on page 3-10. Figure 5-10 shows the circuit diagram and Table 5-2 lists the specifications of the peripheral control output.





| Table 5-2. | Start In | input | circuit | specifications |
|------------|----------|-------|---------|---|
| | 0.00.0 | | 000 | 000000000000000000000000000000000000000 |

| Low level input voltage | $U_{in} < 0.8 V @ 0.75 mA$ |
|--------------------------|----------------------------|
| High level input voltage | U _{in} > 2.0 V |

Chapter 6 **Operation**

This chapter outlines the checks and cleaning procedures of the Q Exactive GC or Exactive GC system that should be performed every day to ensure the proper operation of your system.

Contents

- "Safety Guidelines for Operation" on page 6-2
- "Before Operating the System" on page 6-3
- "Setting the System in Standby Condition" on page 6-6
- "Shutting Down the System" on page 6-7
- "Starting Up the System after a Shutdown" on page 6-9
- "Resetting the System" on page 6-13
- "Installing the Column" on page 6-14

Safety Guidelines for Operation

When operating the Q Exactive or Exactive GC system, pay attention to the following general safety guidelines.

- **WARNING** Suffocation Hazard. Accumulation of nitrogen gas could displace sufficient oxygen to suffocate personnel in the laboratory. Ensure that the laboratory is well ventilated. Local regulations may require a risk assessment for the workplace.
- **A CAUTION Hazardous Chemicals.** Samples and solvents might contain toxic, carcinogenic, mutagenic, or corrosive/irritant chemicals. Avoid exposure to potentially harmful materials. Always wear protective clothing, gloves, and safety glasses when you handle solvents or samples. Also contain waste streams and use proper ventilation. Refer to your supplier's Material Safety Data Sheet (MSDS) for proper handling of a particular compound.
- **A CAUTION** Hot Surface. The external surface of the ion source housing can become hot enough to burn your skin. Avoid touching the ion source housing when the mass spectrometer is in operation. Allow the ion source to cool to room temperature (approximately 60 minutes) before touching the ExtractaBrite removable ion source.
- ★ CAUTION
 Hot Surface. Touching hot parts of the ion source interface might cause severe burns. During operation of the mass spectrometer, the ExtractaBrite removable ion source might reach temperatures of up to 350 °C, while the GC column transfer line might reach temperatures of up to 400 °C. To let the ion source interface cool down, set the ion source and transfer line temperatures to 25 °C. Wait until the ion source has cooled down to room temperature (for approximately 60 minutes) before you begin working on it. Do not leave the instrument unattended when the covers and front door are removed, exposing the hot source parts. Hot ion source parts might ignite combustible material. Keep combustible materials away from the ion source mount.

Before Operating the System

Every day before starting analyses, verify that the instrument is ready for operation by doing the following:

- Checking the Forepump
- Checking the System Vacuum Levels
- Checking the Disk Space on the Data System
- Checking the Mass Accuracy of the Instrument

NOTICE Accurate results can be obtained only if the system is properly calibrated. ▲

Checking the Forepump

* To check the forepump before use

Make sure that the following conditions are met:

- The forepump is filled with oil.
- It is connected to the power supply.
- The gas ballast is shut.

Checking the Nitrogen Supply

Check the nitrogen supply on the regulator of the nitrogen gas tank or tanks. Make sure that you have sufficient gas for your analysis. Based on 24 hour per day operation, typical nitrogen consumption is 1 L (0.035 ft³) per day. If necessary, replace the tank. Verify that the pressure of nitrogen reaching the mass spectrometer is at 800 ± 30 kPa (8 ± 0.3 bar, 116 ± 4 psi). If necessary, adjust the pressure with the tank pressure regulator.

Continue with "Checking the System Vacuum Levels".

Checking the System Vacuum Levels

For proper performance, your Q Exactive GC or Exactive GC system must operate at the acceptable vacuum levels. Operating the system at poor vacuum levels can cause reduced sensitivity and tuning problems. Check your system for air leaks by checking the system vacuum levels before you begin your first acquisition.



You can check the current pressure values in the Vacuum / Bakeout window of the Tune software. To display the Tune software window, choose **Start > Programs > Thermo Exactive Series > Tune**. The Instrument status LED in the toolbar (see image in margin) turns green when the vacuum levels are sufficient for operating your Exactive Series system. If the LED is not green, you might have an air leak; see "Vacuum Leak" on page 7-5 for instructions.

Continue with "Checking the Disk Space on the Data System".

Checking the Disk Space on the Data System

Periodically verify that your hard disk drive has enough free space for data acquisition. The amount of available disk space is shown in the Disk Space dialog box.

- To determine the amount of available disk space
- From the Home Page window (which is available by choosing Start > Programs > Thermo Xcalibur > Xcalibur), choose Actions > Check Disk Space to open the Disk Space dialog box. The Disk Space dialog box lists the following:
 - Current drive and directory (for example, C:\Xcalibur\system\programs)
 - Number of Mb that are available (free) on the current drive
 - Percentage of the current drive that is available
 - Total capacity of the current drive
- 2. To select another disk drive so that you can determine its disk space, click **Directory**.
- 3. When you have completed this procedure, choose **OK** to close the dialog box.

If necessary, you can free space on the hard disk by deleting obsolete files and by moving files from the hard disk drive to a backup medium. First, copy files to the backup medium. After you have copied the files, you can delete them from the hard disk.

Continue with "Checking the Mass Accuracy of the Instrument".

Checking the Mass Accuracy of the Instrument

Thermo Fisher Scientific recommends checking the mass accuracy before you start working. Follow the procedure described in the QuickStart Guide for your instrument. If the instrument indicates that the tune parameters and calibration parameters are not optimal, Thermo Fisher Scientific recommends tuning and calibrating the Q Exactive GC or Exactive GC mass spectrometer. Follow the procedure described in the QuickStart Guide or Software Manual.

NOTICE *Calibration parameters* are instrument parameters that affect the mass accuracy and resolution. *Tune parameters* are instrument parameters that affect the intensity of the ion signal. ▲

You need to optimize the tune parameters (or change the Tune Method) whenever you change the type of experiment. Refer to the QuickStart Guide for a procedure for optimizing the tune parameters for your experiment.

Setting the System in Standby Condition

The Q Exactive GC or Exactive GC system should not be shut down completely if you are not going to use it for a short period of time, such as overnight or over the weekend. In that case, you can leave the system in Standby condition.

NOTICE Thermo Fisher Scientific recommends leaving the mass spectrometer in Standby overnight to provide the best mass accuracy next day. ▲

To place the Q Exactive GC or Exactive GC system in the Standby condition

1. Wait until data acquisition, if any, is complete.



- 2. In the Tune software window, click the **On/Standby** button to put the instrument in Standby condition. The System LED on the front panel of the mass spectrometer turns yellow when the system is in Standby condition.
- 3. Leave the GC power On.
- 4. Leave the autosampler power On.
- 5. Leave the data system power On.
- 6. Leave the Q Exactive GC or Exactive GC main power circuit breaker switch in the On position.

Shutting Down the System

The Q Exactive GC or Exactive GC system does not need to be shut down completely if you are not going to use it for a short period of time, such as overnight or over a weekend. See "Setting the System in Standby Condition" on page 6-6. This section describes how to shut down the system for a maintenance or service procedure.

NOTICE Although removing power abruptly by placing the *main power circuit breaker switch* (see Figure 3-5 on page 3-9) in the Off (O) position will not harm any component within the system, this not the recommended shutdown procedure to follow. ▲

To shut down the Q Exactive GC or Exactive GC system

- 1. Wait until data acquisition, if any, is complete.
- 2. Set heated zones to room temperature on the GC transfer line and the MS transfer line.



- 3. In the Tune software window, click the **On/Standby** button to put the instrument in Off condition. (See image in margin.) All high voltages are shut off, as is the C-Trap and HCD gas.
- 4. Place the electronics service switch, located on the power panel (See Figure 3-5 on page 3-9.), in the Service Mode position.
- 5. Put the main power circuit breaker switch of the mass spectrometer in the Off position.
- 6. Shut down the TRACE 1310 GC. See the GC user documentation for instructions.

WARNING High Voltage. Hazardous electric voltage capable of causing an electric shock is used in the instrument. To ensure that the instrument is free from all electric current, always disconnect the power cords of *mass spectrometer and forepump* before attempting any type of maintenance.

If you are planning to perform routine or preventive system maintenance on the mass spectrometer only, you do not need to turn off the autosampler or data system. In this case, the shutdown procedure is completed. However, if you do not plan to operate your system for an extended period of time, you might want to turn off the autosampler and data system. **NOTICE** An instrument that is shut down still consumes nitrogen because the vent valve is connected to the nitrogen supply of the laboratory. Keeping the nitrogen flow on prevents humidity from contaminating the vacuum system of the mass spectrometer. You may however switch off the nitrogen if your supply is limited. ▲

Starting Up the System after a Shutdown

To start up the Q Exactive GC or Exactive GC mass spectrometer after it has been shut down (and vented), you need to do the following:

- 1. Start up the instrument
- 2. Set up conditions for operation

Starting Up the Instrument

* To start up the Q Exactive GC or Exactive GC system

- 1. Start up the GC and autosampler as is described in the manual that came with the GC and autosampler.
- 2. Switch on data system and monitor as described in the manuals that came with them. Wait until the operating system of the computer is completely loaded.
- 3. To start the Tune software on the data system computer, choose **Start > Programs > Thermo Exactive Series > Tune**.

NOTICE The data system must be running before you start up the instrument. The instrument will not operate until software is received from the data system. ▲

- 4. Turn on the nitrogen flow at the tank, if it is off.
- 5. Make sure that the main power circuit breaker switch is in the Off (O) position and that the electronics service switch is in the Service Mode position.
- Place the main power circuit breaker switch in the On (|) position.
 When you place the main power circuit breaker switch in the On (|) position, the forepump and the turbomolecular pumps are started. All LEDs on the mass spectrometer front panel are off.
- 7. Set the power to the GC to On after the mass spectrometer. This allows the GC to properly identify the auxiliary temperature module controlling the GC transfer line.

When the vacuum system is switched on, the following occurs:

a. After the main switch is switched On, the pumps of the mass spectrometer are run up. To monitor the vacuum readings in the Tune software, it is necessary to switch on the electronics switch, too. The Pirani gauge (see "Vacuum Gauges" on page 3-13) monitors the pressure at the forepump. Within a short time, a significant pressure decrease must be observed. The quality of the vacuum can be estimated by means of the rotation speed of the TMPs (for example, 80% after 15 minutes).

b. If the working pressure is not reached after a preset time, the complete system is switched off.

NOTICE The vacuum control board triggers an alert in the Tune software when a vacuum failure has occurred. ▲

c. The Ion Gauge 1 (IKR 251) is switched on only after the source TMP has exceeded 90% of its maximum rotation speed for five minutes. To extend its life time, this ion gauge is switched off automatically after 30 minutes.

NOTICE For diagnostic purposes, the ion gauge can be switched on manually in the instrument status view of the Tune software. ▲

If the pressure exceeds 1E-4 mbar for more than 10 seconds, the ion gauge is switched off. After five minutes, the ion gauge is switched on again. After three failed attempts, it is only possible to switch on Ion Gauge 1 manually in the Tune software.

d. The Ion Gauge 2 (IKR 270) is switched on only after both TMPs have exceeded 90% of their maximum rotation speed for five minutes. It is then used to monitor the vacuum in the Orbitrap analyzer.

If the pressure exceeds 1E-4 mbar for more than 10 seconds, the ion gauge is switched off. After five minutes, the ion gauge is switched on again. After three failed attempts, it is only possible to switch on Ion Gauge 2 manually in the Tune software.

- e. The Vacuum LED on the system panel turns green when all the following conditions are met:
 - In the Tune software, all LEDs are green. (The Ion Gauge 1 is allowed to be off).
 - Analyzer temperature is below 45 °C.
 - Both TMP frequencies have exceeded 90% of their maximum rotation speed.
- f. When the vacuum measured by the Ion Gauge 2 is better than 1E-8 mbar, the power supplies of the high voltage electronics and the capillary heater are switched on.

NOTICE If both ion gauges are defective, it is not possible to switch on the RF voltage and the high voltages. ▲

- 8. Allow the mass spectrometer to pump down for 5 minutes.
- 9. Place the electronics service switch in the Operating Mode position. See Figure 3-5 on page 3-9. When the electronics service switch is in the Operating Mode position, the following occurs:
 - a. Power is provided to all electronic boards. (The main RF voltage and transfer multipole RF voltage remain off.)
 - b. The internal computer reboots. After several seconds, the Status LED on the front panel turns yellow to indicate that the data system has started to establish a communication link.
 - c. After several more seconds, the Status LED turns green to indicate that the data system has established a communication link. Software for the operation of the instrument is then transferred from the data system to the instrument.
 - d. After approximately 3 minutes, the System LED turns yellow to indicate that the software transfer from the data system is complete.

Start the GC or autosampler (if present) it as is described in the manual that came with the GC or autosampler. After the GC and autosampler are powered on, go to "Setting Up Conditions for Operation" below.

Setting Up Conditions for Operation

To set up your Q Exactive GC or Exactive GC mass spectrometer for operation

- Operation of the system with excessive air and water in the vacuum manifold can cause reduced sensitivity and tuning problems. Before you begin data acquisition with your Q Exactive GC or Exactive GC system, you need to bake out the system for at least twelve hours plus a cooling period of three hours. See "Baking Out the System" on page 8-11.
- After having performed a system bakeout, make sure in the Vacuum/Bakeout window of the Tune software that the UHV pressure is < 1E-8 mbar. Also make sure that the FV pressure is in the < 6E-2 mbar region. Compare the values of the other parameters in the instrument status window with values that you recorded previously.
- 3. Make sure that the gas pressure is within the operational limits:

Nitrogen: 800 ± 30 kPa (8 ± 0.3 bar, 116 ± 4 psi)

See also "Before Operating the System" on page 6-3 for additional information.

Introducing Samples into the Q Exactive GC or Exactive GC Mass Spectrometer

The Q Exactive GC or Exactive GC mass spectrometer, the GC, and the autosampler (if present) have been installed by a Thermo Fisher Scientific field service engineer.

The QuickStart Guide for your instrument gives an introduction on setting up and using the Q Exactive GC or Exactive GC mass spectrometer.

Consider the following safety guideline when introducing sample into the Q Exactive GC or Exactive GC mass spectrometer.

A CAUTION Hazardous Chemicals. Samples and solvents might contain toxic, carcinogenic, mutagenic, or corrosive/irritant chemicals. Avoid exposure to potentially harmful materials. Always wear protective clothing, gloves, and safety glasses when you handle solvents or samples. Also contain waste streams and use proper ventilation. Refer to your supplier's Material Safety Data Sheet (MSDS) for proper handling of a particular compound.

Performing Mass Spectrum Measurements

The QuickStart Guide gives an introduction on performing mass spectrum measurements with the Q Exactive GC or Exactive GC mass spectrometer.

Consider the following safety guidelines when performing measurements with the Q Exactive GC or Exactive GC mass spectrometer.

WARNING Suffocation Hazard. Accumulation of nitrogen gas could displace sufficient oxygen to suffocate personnel in the laboratory. Ensure that the laboratory is well ventilated. Local regulations may require a risk assessment for the workplace.

Resetting the System

If communication between the mass spectrometer and data system computer is lost, it may be necessary to reset the system using the Reset button of the Q Exactive GC or Exactive GC mass spectrometer.

* To reset the system

- 1. Ensure that mass spectrometer and data system computer are both powered on and the mass spectrometer is in Standby condition. See page 6-6 for instructions about placing the instrument to Standby condition.
- 2. To reset the mass spectrometer, press the Reset button located on the power panel. See Figure 3-5 on page 3-9. Make sure the Status LED is extinguished before releasing the Reset button. When you press the Reset button, the following occurs:
 - a. An interruption of the embedded computer causes the CPU to reboot. All LEDs on the front panel are off except the Power LED.
 - b. After several seconds, the Status LED turns yellow to indicate that the data system and the instrument are starting to establish a communication link.
 - c. After several more seconds, the Status LED turns green to indicate that the data system and the instrument have established a communication link. Software for the operation of the instrument is then transferred from the data system to the instrument.

After 3 minutes, the software transfer is complete. The System LED turns either green to indicate that the instrument is functional and the high voltages are on, or yellow to indicate that the instrument is functional and it is in Standby condition.

NOTICE If resetting the system does not resolve the failure: Put the electronics switch in the Service Mode position for about one minute. Afterwards, place the electronics service switch back in the Operating Mode position. ▲

Installing the Column

Check the column for leaks and perform a column evaluation if needed before inserting it into the MS transfer line.

* To check the column for leaks

- On the TRACE 1310, select the Leak Check icon in the Maintenance menu. Otherwise, perform the leak check through the Chromatography Data System. Refer to the *TRACE 1300 and TRACE 1310 Series GC User Guide* for instructions.
- 2. Start the leak check:

The split and purge valves of the selected channel are automatically closed, and the channel is pressurized with carrier gas to the leak check set point.

The system monitors the pressure for one minute. If the pressure does not drop more than the maximum allowed sensitivity value, then the leak check will pass. If the leak check does not pass, use the leak detector to find and fix any leaks.

NOTICE Leaks can be caused by not tightening the fitting on the column flowmeter connector. Check the fitting before looking for the leak elsewhere. ▲

NOTICE INSTRUMENT DAMAGE: Do not allow the column flowmeter connector to exceed 80 °C (176 °F). Otherwise, it will melt and damage the instrument. ▲

- 3. Repeat the leak check until no leaks are indicated.
- 4. Calibrate the carrier gas flow (column evaluation):

a. Carefully push the capillary column end into the flowmeter section of the column flowmeter connector.



Figure 6-1. Connecting the Column to the Flowmeter

- b. Connect the flowmeter to the dedicated fitting on the column flowmeter connector.
- c. If you have a TRACE 1310, select the Back or Front Column icon in the Configuration menu. Otherwise, perform the column evaluation through the Chromatography Data System. See the TRACE 1300 and TRACE 1310 User Guide for instructions.
- d. Select Column and input the column's physical characteristics.
- e. If a pre-/post column is present, set the length and nominal internal diameter of the pre-/post column in the same valid ranges for the column. The following two lines are added to the menu.

NOTICE For the most reproducible results, you should conduct a more detailed column evaluation. However, the following steps, while recommended, are not required. ▲

- f. Start the column evaluation. According to the physical characteristics of the column, the system calculates and displays the relevant column K-factor. At the end of the routine, a message will indicate that the evaluation was successful.
- g. Expect a K-factor of approximately 0.7–0.9 for a 15 m, 0.25 mm i.d. column (1.3–2.0 for a 30 m, 0.25 mm i.d. column). If the column does not report a K-factor within this range or within 0.1 units of the previous stored value, check for a leak or broken column using the leak detector. The K-factor is a

measured resistance for the column. A K-factor that is too low may indicate a leak in the system, while a K-factor that is too high may indicate a blockage.

Fix any issues found and rerun column evaluation until an appropriate K-factor is achieved.

- 5. Disconnect the column flowmeter.
- 6. Disconnect the column from the column flowmeter connector.
- 7. Remove the clear plastic component, including its fittings, from the oven and set them aside.
- * To install the column in the Q Exactive GC or Exactive GC system
- 1. In Tune, place the instrument in the Off state.
- 2. Cool the oven, transfer line and source:
 - a. On the GC, set the Oven to **Off**.
 - b. On the GC, in the Auxiliary Temperature Control, set Transfer Line 1 and Transfer Line 2 to **Off**.
 - c. In Tune Instrument Control EI/CI source, set the:
 - i. MS transfer line temp to 40 °C.
 - ii. Ion source temp to 175 °C (to avoid excessive oxidation of source parts or contamination from the source plug).
- 3. Using the source removal tool and vacuum interlock, remove the ion source. (See "Removing the Ion Source Cartridge from the Q Exactive GC or Exactive GC System" on page 8-15 for correct use of the vacuum interlock and source insertion/removal tool.)

4. Place the ion source cartridge on the source holder and set aside.



Figure 6-2. Storing the Ion Source Cartridge in the Source Holder

5. Place the source plug in the source plug holder.



Figure 6-3. Attaching the Source Plug to the Source Plug Holder

6. Attach the source exchange tool to the source plug in the source plug holder.





7. Twist the plug until it aligns securely in the grooves in the source exchange tool and remove the plug from the holder



Figure 6-5. Attaching the Source Plug to the Source Exchange Tool

NOTICE IMPORTANT Use compressed air to blow all the dust off the source plug before inserting it into the mass spectrometer.

8. Once the ion source temperature has dropped below 200 °C, insert the barrel end of the source exchange tool into the vacuum interlock

and twist it clockwise to lock it into position. Be sure the black handle remains fully extended and locked.

Figure 6-6. Inserting the Source Plug into the Vacuum Interlock

- 9. Evacuate the VPI.
 - a. Confirm that the source removal tool is properly engaged in the VPI.
 - b. Press the blue Evacuate button on the front of the instrument.
 - c. The Evacuate light will begin to flash green, and should continue to flash green for approximately 20 seconds.
 - d. If the pressure has returned to an acceptable value after the 20-30 second wait, the evacuate light will turn off and the Ready to Open light will be solid green. At that point, the air has been evacuated from the instrument and it is safe to open the vacuum interlock value.
- 10. Pull the vacuum interlock handle up when the Ready to Open light is a solid green.
- 11. Twist the handle of the tool slightly to the left until it is feels like it is lodged into the left-most track.
- 12. Push the handle toward the instrument until the end of the handle aligns with the engraved line at the end of the barrel. When you reach this line, the tool is all the way in and the source plug is securely placed in the instrument.

NOTICE IMPORTANT The source plug should remain attached to the source exchange tool. Do not rotate the source exchange tool handle to attempt to disengage the source plug.



Figure 6-7. Raising the Vacuum Interlock Handle

- 13. Wait for oven and transfer line temperatures to drop below 50 °C to avoid burns before proceeding to touch the column and nut.
- 14. Use the GC transfer line handle to slide the GC transfer line away from the MS transfer line.



Figure 6-8. Separating the GC and MS Transfer Lines

15. Remove the current column and nut if present.

NOTICE Monitor the foreline pressure when removing the column and nut to confirm that the source plug is properly sealing the transfer line. If the pressure exceeds 3 mbar, the leak is excessive, and the source plug should be reseated or inspected for damage. If the turbomolecular pump is forced off by the vacuum protection and the pump speed drops below 80% speed, cycling power will not restart the turbomolecular pump. The pump speed must further drop below 25% before cycling the power to reset the pump and allow it to spin up to 100%. Be careful not to have the circuit breaker off for more than 5 seconds or there is a risk that the system will vent and must be pumped down overnight. \blacktriangle

16. Unwind an appropriate column length to insert into the transfer line along the front of the instrument. Leaving about an inch gap between the column and the left side of the front panel will usually give you an appropriate length of column for installation.

Column Gap



Figure 6-9. Measuring the Column Length



17. Insert the new column through the GC transfer line.

Figure 6-10. Inserting the New Column through the GC Transfer Line

18. Carefully extend the column out the front to allow application of the nut and ferrule.



Figure 6-11. Extending the Column to the Front of the Instrument

- 19. Insert the column through the nut and ferrule (flat side of the nut faces the MS).

Figure 6-12. Inserting the Column through the Nut and Ferrule

- 20. Use a scoring wafer to score and then remove the last 10 mm of column to provide a clean, well-cut end.
- 21. Wipe the column with an alcohol soaked-wipe after inserting through the ferrule.



Figure 6-13. Scoring and Cutting the Column

22. Carefully push the column back into the GC transfer line while keeping the nut and ferrule on the column.



Figure 6-14. Proper Placement of the Column in the GC Transfer Line

23. Insert the column into the MS transfer line and tighten the nut until the column just resists sliding through the ferrule.



Figure 6-15. Inserting the Column into the MS Transfer Line

- 24. Loosen the nut ¼ turn and push the column into the MS transfer line until it just touches the source plug.
- 25. Pull the column $\frac{1}{2}$ to 1 mm away from the source plug and tighten the nut $\frac{1}{2}$ turn.

NOTICE To avoid forcing the column into the source plug when tightening the nut, the column can be pulled back approximately 1 mm before tightening the nut. ▲



Figure 6-16. Tightening the Nut

26. Ensure the column and nut are correctly installed in the MS transfer line.



Figure 6-17. Correctly Installed Column in MS Transfer Line

27. Pull the GC transfer line handle to the left to close it.



Figure 6-18. Closed MS Transfer Line

- 28. Remove the source plug with the insertion/removal tool.
- 29. Lower the handle to close the vacuum interlock.
- 30. Remove the source exchange tool.
- 31. Allow the source plug to cool.
- 32. Carefully remove the source plug from the insertion/removal tool using the source plug holder.

NOTICE Tip To avoid collecting dust on the source plug, store it in a closed container when not in use. \blacktriangle

- 33. Using the source holder, place the ion source on the insertion/removal tool and install the ion source using the vacuum interlock.
- 34. In Tune Instrument Control > EI/CI Source, set the:
 - a. MS transfer line temp to the method temperature.
 - b. Ion source temp to the method temperature.
- 35. In Tune, place the instrument in the On state.
- 36. Leak check at the nut with tetrafluoroethane spray and tighten with a 1/4" wrench as needed. Perform leak checking by scanning in full scan and looking for +CF₃ (68.99466) and +CH₂CF₃ (83.01031) peaks while spraying potential leak spots with tetrafluoroethane (dusting spray or refrigerant R-134A).)
- 37. Confirm the GC transfer line is covering the nut to prevent a cold zone on the column.
- 38. If vacuum compensation was set to **Off** for any reason (such as conditioning a new column), set vacuum compensation to **On**.
- 39. On the GC, set the Oven to **On**.
- 40. On the GC, in the Auxiliary Temperature Control, set Transfer Line 1 and Transfer Line 2 to **On**.
- 41. If necessary, reinsert the ion source to assure good electrical contacts using the insertion/removal tool and vacuum interlock once all temperatures have stabilized for 30 minutes and the source has thermally expanded.
- 42. Replace the vacuum interlock knob and evacuate the inlet valve chamber to remove the remaining air between the ball valve and interlock plug.
- 43. Confirm there are no leaks before beginning any tuning or analyses.

Chapter 7 Troubleshooting

This chapter provides information about identifying and solving common problems with Q Exactive GC and Exactive GC mass spectrometers.

Contents

- "Safety Guidelines for Troubleshooting" on page 7-2
- "Fault Table" on page 7-3
- "Main Power Failure" on page 7-4
- "Vacuum Leak" on page 7-5
- "Failure of UHV Chamber Heating Control" on page 7-7
- "Turbomolecular Pump is Not Running" on page 7-8

Safety Guidelines for Troubleshooting

When performing troubleshooting on the Q Exactive GC or Exactive GC system, pay attention to the following general safety guidelines.

- ▲ WARNING High Voltage. High voltages capable of creating an electric shock are used in the instrument. Do not remove protective covers from PCBs. Opening the instrument housing is only allowed for maintenance purposes by Thermo Fisher Scientific personnel. To ensure that the instrument is free from all electric current, always disconnect the power cords of *mass spectrometer and forepump* before attempting any type of maintenance.
- ★ CAUTION
 Hot Surface. Touching hot parts of the ion source interface might cause severe burns. During operation of the mass spectrometer, the ExtractaBrite removable ion source might reach temperatures of up to 350 °C, while the GC column transfer line might reach temperatures of up to 400 °C. To let the ion source interface cool down, set the ion source and transfer line temperatures to 25 °C. Wait until the ion source has cooled down to room temperature (for approximately 60 minutes) before you begin working on it. Do not leave the instrument unattended when the covers and front door are removed, exposing the hot source parts. Hot ion source parts might ignite combustible material. Keep combustible materials away from the ion source mount.
- ▲ CAUTION Hot Surface. Touching hot parts of the forepump might cause burns. The forepump in function is hot and some surfaces could reach a temperature higher than 70 °C (158 °F). Switch off the pump and let it cool down before any intervention or take appropriate precautions. Always wear heat protective gloves when working on a pump that is "still warm from operation".
 - Service by the customer must be performed by trained qualified personnel only and is restricted to servicing mechanical parts. Service on electronic parts must be performed by Thermo Fisher Scientific field service engineers only.

Never try to repair or replace any component of the system that is not described in this manual without the assistance of your Thermo Fisher Scientific field service engineer.

Fault Table

If malfunctions on the mass spectrometer occur, you will find possible causes and instructions for repair in Table 7-1.

| Problem | Possible Causes | Remedy |
|--|--|----------|
| Tune software shows bad vacuum | System was vented because of a mains failure | page 7-4 |
| | Vacuum leak | page 7-5 |
| Temperature of UHV chamber is higher than expected | UHV chamber heating control has failed | page 7-7 |
| Turbomolecular pump is not running | TMP is switched off because of overheating | page 7-8 |

Table 7-1.Troubleshooting

Main Power Failure

A main power failure has the same consequence as switching off with the main power circuit breaker switch. If the power is available again, the system is started up automatically: the pumps are switched on and the vacuum is created. If the system has been vented during the mains failure, it is necessary to bake out the system to obtain the operating vacuum. See "Baking Out the System" on page 8-11.

If the log file of the data system shows a reboot of the system and the pressure reading in the Tune software shows a bad vacuum, this indicates that the system was vented. In case of frequent but short power failures we recommend installing an uninterruptible power supply (UPS). If main power failures occur frequently while the system is not attended (for example, in the night), we recommend installing a power fail detector.

Vacuum Leak

For proper performance, your Q Exactive GC or Exactive GC system must operate at acceptable vacuum levels. You can check the current pressure values in the Vacuum / Bakeout window of the Tune software window.

To check the vacuum levels

- To display the Tune software window, choose Start > Programs > Thermo Exactive Series > Tune. The Instrument status LED in the toolbar (see image in margin) turns green when the vacuum levels of the instrument are sufficient for operating your Q Exactive GC system.
- 2. In the Tasks panel of the Tune software window, click

Vacuum / Bakeout to display the Vacuum / Bakeout window. See Figure 7-1. Green LEDs indicate that the readback values are sufficient for operating the Q Exactive GC mass spectrometer.

| A.I. | |
|---|-----|
| 👻 Vacuum / Bakeout 👘 | |
| Fore vacuum (mbar) 4.83E-02 UHV (mbar) 4.16E-10 | 3 |
| Bakeout time (h) | 4.0 |
| Enter standby after Bakeout M | |
| Bake out Stop Help | |
| | |



3. Compare the current values of the pressures in the vacuum manifold with the values listed in Table 7-2. If the current values are higher than normal, there might be an air leak.

| Gauge type | Name in Tune software | Typical values |
|--------------|--------------------------|------------------|
| Pirani | Fore Vacuum | about 5E-02 mbar |
| Cold cathode | High Vacuum ^a | about 3E-05 mbar |
| Cold cathode | Ultra High Vacuum | < 8E-10 mbar |

^a This parameter is visible only when the ion gauge in the high-vacuum chamber is switched on. Refer to the Tune Help for details.

4. If the pressure in the Ultra High Vacuum region is high (above 1E-9 mbar), the instrument needs to be baked out for about

10 hours or more. See "Baking Out the System" on page 8-11 for instructions on performing a system bakeout.

If the pressure remains high, the system might have an air leak. See below for instructions.

* To check the system for major air leaks

Listen for a rush of air or a hissing sound inside the mass spectrometer.

Possible causes of a major leak might be a loose or disconnected fitting, an improperly positioned O-ring, or an open valve. If you suspect an air leak in the forevacuum region, check the vacuum tube for holes. Also check the clamp that fixes the vacuum tube to the forevacuum port (elbow) of the mass spectrometer. See Figure 3-6 on page 3-11. It might be loose because the forepump was shifted or the vacuum tube is twisted.

✤ To fix an air leak

- 1. Shut down the system; see "Shutting Down the System" on page 6-7.
- 2. Make a visual inspection of the vacuum system and vacuum lines for leaks.
- 3. Check each fitting and flange on the system for tightness, and tighten the fittings or flanges that are loose.

Do not tighten fittings indiscriminately. Pay particular attention to fittings that have been changed recently or to fittings that have been subjected to heating and cooling.

- 4. Ensure that the o-rings and the cover plates of the vacuum manifold are properly positioned.
- 5. Ensure the MS transfer line nut is secure. A leak can develop at this seal when the GC transfer line temperature is reduced significantly.
- 6. Confirm the GC capillary column is not broken or that the vacuum interlock is properly sealed.
- 7. Ensure that the glass cover of the ion source is properly seated on the o-ring if source maintenance has been performed with the covers off

If you cannot find the location of the leak or tighten the leak yourself, contact your Thermo Fisher Scientific field service engineer.

Failure of UHV Chamber Heating Control

During general operation of the mass spectrometer, the temperature of the UHV chamber is not regulated. Only during a system bakeout, electric power is supplied to the heating elements of the UHV chamber. The heating always operates at maximum power. Thus, failure of the heating control does not lead to a dangerous overheating of the mass spectrometer.

If the Q Exactive GC or Exactive GC mass spectrometer does not work as expected, use the Tune software for error diagnosis:

• The messages window displays real-time information about the statuses of the instrument, the control service, or other programs. If the heating was terminated, the window displays a corresponding error message.

In case of a failure of the UHV chamber heating control, shut down the mass spectrometer as described on page 6-7. To prevent permanent damage to components of the Q Exactive GC mass spectrometer, Thermo Fisher Scientific recommends calling a Thermo Fisher Scientific field service engineer.

Turbomolecular Pump is Not Running

A turbomolecular pump may be switched off because of one of the following reasons:

- Turbomolecular pump is blocked
- Failure of fans in turbomolecular pump

Each of the above reasons might lead to an overheating of the pump. When overheated, a turbomolecular pump switches off automatically to prevent its destruction. This overheating protection prevents the outbreak of a fire and minimizes the risk of destroying the pump.

If the Q Exactive GC or Exactive GC mass spectrometer does not work as expected, use the Tune software for error diagnosis:

- The instrument status window displays real-time status information for the instrument components. All parameters are arranged in a tree view. In addition to showing numerical values of parameters (for example, pump speeds or component temperatures), the instrument status window uses icons to indicate the statuses of system components.
- The messages window displays real-time information about the statuses of the instrument, the control service, or other programs. It might display additional information.

In case of an overheated turbomolecular pump, shut down the mass spectrometer as described on page 6-7. To prevent permanent damage to components of the Q Exactive GC or Exactive GC mass spectrometer, Thermo Fisher Scientific recommends calling a Thermo Fisher Scientific field service engineer.

Chapter 8 Maintenance

This chapter describes routine maintenance procedures that must be performed to ensure optimum performance of the Q Exactive GC or Exactive GC mass spectrometer.

Contents

- "Safety Guidelines for Maintenance" on page 8-2
- "General Advice for Maintenance" on page 8-4
- "Inspection- and Servicing Plan" on page 8-5
- "Maintaining the Vacuum System" on page 8-8
- "Maintenance of the Fan Filters" on page 8-13
- "EI/CI Source Maintenance" on page 8-15
- "Maintaining GCs or Autosamplers" on page 8-50
- "Consumables" on page 8-51
- "Thermo Fisher Scientific Service" on page 8-52

Safety Guidelines for Maintenance

When performing maintenance on the Q Exactive GC or Exactive GC system, pay attention to the following general safety guidelines.

▲ WARNING High Voltage. High voltages capable of causing an electric shock are used in the instrument. Do not remove protective covers from PCBs. Opening the instrument housing is only allowed for maintenance purposes by Thermo Fisher Scientific personnel. To ensure that the instrument is free from all electric current, always disconnect the power cords of *mass spectrometer and forepump* before attempting any type of maintenance.

▲ CAUTION Hot Surface. Touching parts of the forepump might cause burns. The forepump in function is hot and some surfaces could reach a temperature higher than 70 °C (158 °F). Switch off the pump and let it cool down before any intervention or take appropriate precautions. Always wear heat protective gloves when working on a pump that is "still warm from operation". Take note of the warning labels on the pump.

▲ CAUTION Hot Surface. Touching hot parts of the ion source interface might cause severe burns. During operation of the mass spectrometer, the ExtractaBrite removable ion source might reach temperatures of up to 350 °C, while the GC column transfer line might reach temperatures of up to 400 °C. To let the ion source interface cool down, set the ion source and transfer line temperatures to 25 °C. Wait until the ion source has cooled down to room temperature (for approximately 60 minutes) before you begin working on it. Do not leave the instrument unattended when the covers and front door are removed, exposing the hot source parts. Hot ion source parts might ignite combustible material. Keep combustible materials away from the ion source mount.

A CAUTION Hazardous Chemicals. Samples and solvents might contain toxic, carcinogenic, mutagenic, or corrosive/irritant chemicals. Avoid exposure to potentially harmful materials. Always wear protective clothing, gloves, and safety glasses when you handle solvents or samples. Also contain waste streams and use proper ventilation. Refer to your supplier's Material Safety Data Sheet (MSDS) for proper handling of a particular compound.



It is the user's responsibility to maintain the system properly by performing the system maintenance procedures on a regular basis.

Service by the customer must be performed by trained qualified personnel only and is restricted to servicing mechanical parts. Service on electronic parts must be performed by Thermo Fisher Scientific field service engineers only.

Never try to repair or replace any component of the system that is not described in this manual without the assistance of your Thermo Fisher Scientific field service engineer.

Only use fuses of the type and current rating specified. Do not use repaired fuses and do not short-circuit the fuse holder.

General Advice for Maintenance

When performing maintenance on the Q Exactive GC or Exactive GC mass spectrometer, observe the following advice:

- Accurate results can be obtained only if the system is in good condition and properly calibrated.
- Preventive maintenance must commence with installation, and must continue during the warranty period to maintain the warranty. Thermo Fisher Scientific offers maintenance and service contracts. Contact your local Thermo Fisher Scientific office for more information. Routine and infrequent maintenance procedures are listed in Table 8-1.
- The user maintenance procedures described in this manual do not require removing the instrument housing. Thermo Fisher Scientific assumes no responsibility and will not be liable for instrument damage and/or operator injury that might result from using the instrument without the housing attached. Therefore, a Thermo Fisher Scientific field service engineer must be called if removal of the instrument housing is required.
- To successfully carry out the procedures listed in this chapter, observe the following rules:
 - Proceed methodically
 - Always wear clean, talc-free, and lint-free gloves when handling internal components of the Q Exactive GC or Exactive GC system. See "Personal Protective Equipment" on page 4-11 for a specification for the required gloves.
 - Always place the components on a clean, lint-free surface.
 - Never overtighten a screw or use excessive force.
 - Dirty tools can contaminate your system. Keep the tools clean and use them exclusively for maintenance and service work at the mass spectrometer.
 - Never insert a test probe (for example, an oscilloscope probe) into the sockets of female cable connectors on PCBs.

Inspection- and Servicing Plan

Routine and infrequent maintenance procedures to be performed by the user are listed in Table 8-1.

| MS Component | Procedure | Frequency | Procedure Location |
|--------------|------------------------------------|--|----------------------------------|
| Instrument | System bakeout | If necessary (for example, after performing maintenance work on the vacuum system) | page 8-11 |
| | Check warning labels on instrument | Annually | page 8-6 |
| | Leak check gas lines | Annually | page 8-7 |
| Cooling fans | Check fan filters | Every 4 weeks | page 8-13 |
| | Clean fan filters | If necessary | - |
| Forepump | Purge (decontaminate) oil | As needed | See manufacturer's documentation |
| | Check oil level | Monthly | page 8-9, see also |
| | Check oil condition | Depends on process | manufacturer's |
| | Add oil | If oil level is low | |
| | Check gas ballast valve | Monthly | - |
| | Clean dirt trap | Monthly | - |
| | Change oil | Every 3000 h (~4 months) of operation ^a | - |
| | Replace exhaust filter | If oil mist appears at exhaust or annually | - |
| | Check anti-suckback valve | Annually | - |
| | Clean fan guard | Annually | - |

 Table 8-1.
 User maintenance procedures

^a The forepump oil may be changed less frequently depending on sample throughput and type.

Returning Parts

To protect our employees, we ask you for some special precautions when returning parts to the factory for exchange or repair. Your signature on Health and Safety Form confirms that the returned parts have been de-contaminated and are free of hazardous materials. See "Safety Advice for Possible Contamination" on page 8-52 for further information.

Cleaning the Surface of the Instrument

Clean the outside of the instrument with a dry cloth. For removing stains or fingerprints on the surface of the instrument (panels, for example), slightly dampen the cloth (preferably made of microfiber) with distilled water.

NOTICE Prevent any liquids from entering the inside of the instrument. Leaking liquids might get into contact with electronic components and cause a short circuit. ▲

Checking Warning Labels

Safety warnings on mass spectrometer and other devices of the GC/MS system must always be complete, clearly visible and legible.

In addition to the safety instructions that can be found throughout this manual, various warning labels on the instrument inform the user about possible hazards (for example, caused by hot surfaces or high voltage). See "Safety Symbols on the Instrument" on page 4-3 for an overview. To protect all personnel coming near the instrument, annually make sure that all warning labels on the instrument are still present. If warning labels are missing or unreadable, contact a Thermo Fisher Scientific field service engineer for replacements. Also check the warning labels on forepump and other devices of the GC/MS system.

Leak-Checking Gas Lines

Regularly leak check each gas line from the gas supply in the laboratory to the instrument.

* To perform a leak check for a gas line

- 1. After closing all valves in the instrument, monitor the manometer of the gas regulator for some minutes.
- 2. If the pressure falls significantly (for example, the nitrogen pressure falls by more than 10 psi / 690 mbar within two minutes), you should search for leaks in the gas line. This nitrogen pressure test cannot be performed when the instrument is powered off because the nitrogen is freely flowing through the vent valve.
- 3. Search for leaks in the gas line, for example, by using a conventional thermal conductivity-based leak detector, such as is widely used to check leaks in gas chromatography equipment.

NOTICE These leak detectors will not detect nitrogen levels. ▲

NOTICE When the Q Exactive GC or Exactive GC system is in the **On** or **Standby** state, nitrogen is consumed at approximately 6 mL/min. The system should be placed in the **Off** state for pressure checks. ▲

- 4. If you detect a leak (which is usually at a connection), verify the tightness of the connection. In case of doubt, replace it.
- 5. When you cannot find a leak in the gas line, we recommend calling a Thermo Fisher Scientific field service engineer to check for gas leaks within the instrument.

Maintaining the Vacuum System

This section describes maintenance procedures for the vacuum pumps and the vacuum manifold of the Q Exactive GC or Exactive GC mass spectrometer.

Pumps Maintenance

This section only outlines the maintenance procedures for the forepump and the turbomolecular pumps (TMPs) of the mass spectrometer. The manuals of the pump manufacturers give detailed advice regarding safety, operation, maintenance, and installation. Note the warnings and precautions contained in these manuals!

Maintenance of the Forepump

The foreline (roughing) pump is usually located on the floor behind the Q Exactive GC or Exactive GC instrument and occasionally requires maintenance. It establishes the vacuum needed to run the turbomolecular pump inside the instrument. Typically, the foreline pump oil needs to be replaced every four months. However, depending on your sample type and frequency of use, your maintenance interval will be different. Refer to the foreline pump documentation for information. The forepump requires several maintenance procedures to be performed by the user. Table 8-2 outlines the maintenance schedule for the forepump as recommended by the pump manufacturer. To simplify the maintenance work, the pump manufacturer recommends combining several jobs. For maintenance instructions, refer to the forepump manual.

| Maintenance job | Frequency |
|---------------------------|--|
| Check oil level | Monthly |
| Check oil condition | Depends on process |
| Check gas ballast valve | Monthly |
| Change oil | Every 3000 h of operation |
| Replace exhaust filter | If oil mist appears at exhaust or annually |
| Check anti-suckback valve | Annually |
| Clean fan cover | Annually |

| Table 8-2. Maintenance | schedule of the forepump |
|------------------------|--------------------------|
|------------------------|--------------------------|

| Hot Surface. Touching hot parts of the forepump might cause burns. |
|--|
| The forepump in function is hot and some surfaces could reach a |
| temperature higher than 70 °C (158 °F) for GC/MS systems. Switch off |
| the pump and let it cool down before any intervention or take |
| appropriate precautions. Always wear heat protective gloves when |
| working on a pump that is "still warm from operation". Take note of |
| the warning labels on the pump. |
| |

A CAUTION Hot Liquid. Touching hot forepump oil might cause burns. Always wear protective gloves and protective goggles when you handle the forepump oil.

A CAUTION Hazardous Chemicals. The forepump oil might cause skin or eye irritation and it might contain toxic, carcinogenic, mutagenic, or corrosive/irritant chemicals. Avoid exposure to potentially harmful materials. Always wear protective clothing, gloves, and safety glasses when you handle the forepump oil.

When disposing of used oil, observe the relevant environmental regulations! For instructions about proper handling, refer to the Material Safety Data Sheet (MSDS) for the forepump oil.

Forepump oil and exhaust filters are available from Thermo Fisher Scientific (see Chapter 9: "Replaceable Parts"). If you want to order other spare parts, contact the pump manufacturer (Edwards for GC/MS systems).

Maintenance of the Turbomolecular Pumps

This topic outlines the maintenance work for the TMPs. These procedures require removing the housing of the instrument and partially disassembling it. Therefore, a Thermo Fisher Scientific field service engineer must be called if servicing is required. See also page 8-53.

Maintenance of the Source TMP

The pump manufacturer (Pfeiffer Vacuum) recommends changing the operating fluid reservoir every three years at the latest. Depending on the operating conditions, changing in two-year intervals might be necessary. Changing of the TMP bearing is recommended every four years, at least.

Maintenance of the Analyzer TMP

The pump manufacturer (Oerlikon Leybold Vacuum) recommends changing the standard bearing every 45000 operating hours at the latest.

Baking Out the System

The system bakeout of the mass spectrometer removes unwanted gases or molecules (collected or remaining) from the high-vacuum region of the instrument. Ions can collide with those gases or molecules resulting in lower overall sensitivity. Therefore, Thermo Fisher Scientific recommends baking out the instrument if the high vacuum decreases noticeably during routine operation.

Bakeout is mandatory after the system has been vented for maintenance or service work in the analyzer region. You should bake out an instrument that has been vented for at least twelve hours (12 hours) before you can start using it again.

If the system has vented during a power failure and it not at the correct pressure and you need to use the system within 24 hours, it is necessary to bake out the system to attain the operating vacuum. See "Starting Up the System after a Shutdown" on page 6-9.

NOTICE Before you start the bakeout, ensure that the pumps are up and running at their operating speed. If you have just switched on the mass spectrometer, this will take about 10 minutes. See "Starting Up the Instrument" on page 6-9. To check the pump speed, open the Instrument Status window of the Tune software and expand the Vacuum System node of the Instrument tree. ▲

* To perform a system bakeout



- 1. In the Tune software window, click the **On/Standby** button to put the instrument in **Off** condition. (See image in margin.)
- 2. In the Tasks panel of the Tune software window, click

Vacuum / Bakeout to display the Vacuum / Bakeout window. See Figure 8-1.

| <u>~</u> ? |
|---|
| Vacuum / Bakeout |
| Fore vacuum (mbar) 5.18E-02 Image: Constraint of the second seco |
| Bakeout time (h) 4.0 🔤 |
| 0.0 % |
| Bake out Stop Help |

Figure 8-1. Vacuum / Bakeout window

3. Enter the desired baking duration (in hours) into the spin box. The available range is 4 to 30 hours.

4. Click **Bake out**. A dialog box shows the duration of the baking procedure. See Figure 8-2. Click **Yes** to confirm the message.

| Bake ou | t 🛛 | |
|---------|--|--|
| 2 | Bakeout will last 14.0 hours and will be followed by a cooling and stabilization time of about 3 hours. The instrument will be inaccessible for approximately 17 hours. | |
| | Continue? | |
| | Yes No | |

Figure 8-2. Bakeout dialog box

5. The dialog box disappears and the baking procedure starts. The instrument indicates the active bakeout procedure by a flashing Vacuum LED. (See Figure 3-3 on page 3-7.) Additionally, the Tune software displays a corresponding message box. See Figure 8-3.

| Dialog with Thermo Exactive Plus | |
|----------------------------------|--|
| (j) | Instrument procedure running. |
| \checkmark | - Maintainance - Vacuum Bakeout - Heating Phase |
| | Please wait |
| Cance | |



6. The baking of the instrument stops after the preset duration. The Vacuum LED keeps flashing until the cooling and stabilization time (of about 3 hours) is finished.

Click **Stop** in the Vacuum / Bakeout window to abort the baking routine before the preset time.

A CAUTION Hot Surface. Touching hot parts of the instrument immediately after a bakeout might cause burns. If you abort a system bakeout, parts of the instrument can be hot. Allow the instrument to cool for at least three hours before you start operating it again.

Maintenance of the Fan Filters

Each of the two ventilation slots at the rear side of the mass spectrometer is equipped with a fan filter. See Figure 8-4.



Pull here to open





NOTICE Avoid blocking the ventilation slots at the rear of the mass spectrometer. Items might fall behind the instrument, inhibit airflow, and cause the system to overheat. Depending on the circumstances, either the Tune software will switch off the instrument and display an error message or the turbomolecular pump control will shut down the instrument and vent it. \blacktriangle

Checking the Fan Filters

Check the fan filters every four weeks.

* To check the fan filters

- 1. Each fan filter bracket is mounted on hinges. Insert a finger into the recess in the instrument frame and pull at the fan filter bracket to open it. See Figure 8-4 and Figure 8-5.
- 2. Remove each fan filter from the rear of the mass spectrometer by pulling it out of the filter bracket. See Figure 8-5.



Figure 8-5. Removing fan filters from the filter bracket

If the fan filters are covered with dust, proceed as described in "Cleaning the Fan Filters" below. Replacements for the fan filters are available from Thermo Fisher Scientific (see Chapter 9: "Replaceable Parts").

Cleaning the Fan Filters

* To clean the fan filters

- 1. Remove the fan filters as described in "Checking the Fan Filters" above.
- 2. Wash the fan filters in a solution of soap and water.
- 3. Rinse the fan filters with tap water.
- 4. Squeeze the water from the fan filters and allow them to air dry.
- 5. Reinstall the fan filters in the fan filter brackets.

EI/CI Source Maintenance

Removing the Ion Source Cartridge from the Q Exactive GC or Exactive GC System

1. Twist off the round vacuum interlock knob located on the interior front panel and set it aside. There is a vacuum feedthrough with a ball valve that allows access to the ion source without venting the instrument

NOTICE To prevent leaks through the vacuum interlock, the vacuum interlock knob must be attached to the instrument, except when you are removing or inserting the ion source cartridge. After you reattach the knob, press the **Evacuate** button to remove any air inside the vacuum interlock. ▲



Figure 8-6. Locating the Vacuum Interlock Knob and Evacuate Button

2. Get the source exchange tool that shipped with your instrument. It is used to remove and insert the ion source cartridge through the vacuum interlock. The tool has a large black handle on one end and a stainless steel barrel at the other. On the black handle is a diagram describing how to insert and remove the ion source cartridge from the instrument using the tool. The stainless steel barrel is cut with a track and the black handle moves up and over the track, depending on whether you are removing or installing an ion source cartridge.



Figure 8-7. Locating the Vacuum Interlock Knob and Evacuate Button

- 3. Grasp the handle of the source exchange tool in one hand and use your other hand to pull the metal barrel out and away from the handle so that tool is fully extended.
- 4. Attach the source exchange tool to the front of the instrument.
 - a. With your hand around the stainless steel barrel, twist the tool until the alignment groove at the end of the barrel aligns with

the left screw around the slot vacated by the vacuum interlock knob.



Figure 8-8. Inserting the Ion Volume Tool

b. Twist and push the stainless steel barrel to the right until it clicks into place under the screw at the top of the slot.



Figure 8-9. Twisting the Tool into Place

- 5. Evacuate the vacuum probe interlock (VPI). The VPI is located behind the vacuum interlock knob and is accessed by removing the knob.
 - a. Confirm that the source removal tool is properly engaged in the VPI.
 - b. Press the blue **Evacuate** button on the front of the instrument.
 - c. The **Evacuate** light flashes amber and then green as the inlet evacuates and should continue to flash green for approximately 20 seconds.
 - d. If the pressure has returned to an acceptable value after the 20-30 second wait, the evacuate light will turn off and the **Ready to Open** light will be solid green. At that point, the air has been evacuated from the ball valve and it is safe to open the vacuum interlock valve.

NOTICE If the evacuate light flashes for only a short time then returns to a solid light without the **Ready to Open** light turning green, there is a leak in the VPI seal. The source removal tool connection should be checked or field service contacted. \blacktriangle



Figure 8-10. Evacuating the System

6. Twist, then loosen the top part of the vacuum interlock handle to allow the entire handle to swing up and down. This handle controls the interior ball valve, which seals the vacuum chamber.

7. Swing the handle down and then twist the top of it in the opposite direction to lock it into place.

NOTICE Be sure the source exchange tool handle is locked securely before proceeding to the next step (opening the interior ball valve). The locking function is designed to prevent the source exchange tool from being sucked into the manifold when the ball valve is opened. ▲

8. Lift the handle up to open the interior ball valve.

NOTICE If more than 60 seconds have passed since the **Ready to Open** indicator light has come on, it will turn off. You should press the **Evacuate** button and wait until the **Ready to Open** light is lit again before opening the valve. Do not open the valve if the **Ready to Open** light is not on. This may indicate a leak in the valve region. When a leak is detected during the evacuate sequence, the amber evacuate LED will flash on and off. ▲

9. Slowly push the ion cartridge tool into the instrument. Because you are removing the ion volume in this step, you will go down the right side of the metal track on the barrel

NOTICE INSTRUMENT DAMAGE: Make sure the vacuum interlock handle is all the way up. Otherwise if you insert the tool with the handle down, you can damage the instrument. ▲



Figure 8-11. Pushing the Tool into the Instrument

- 10. Once the tool is all the way in (when the groove at the end of the barrel is covered by the black handle) twist the handle to the left to engage the ion source cartridge and move it onto the end of the barrel. You are essentially disconnecting the ion source cartridge from the ion source block and moving it onto the tool.
- 11. Pull the tool toward you and down the left side of the metal track on the barrel. As you keep pulling it toward you, more and more of the barrel will be exposed. You may encounter resistance while removing the source. To release the source from the spring contacts make small repeated rotations (vibrations) of the handle to the left and right quickly.



Figure 8-12. Pulling the Tool Down the Left Track

12. Once you reach the end of the track (when the back line at the end of the barrel is uncovered by the black handle), twist the handle to the left to lock it into place.





13. Pull the vacuum interlock handle down to close the interior ball valve.



Figure 8-14. Pulling Down the Vacuum Interlock Handle

- 14. Twist the end of the vacuum interlock handle and flip the swing handle up so that it rests next to the vacuum interlock knob location. Then twist the end again to hold it in place.
- 15. Replace the plug in the VPI to prevent accidental venting and excessive leaks.

NOTICE INSTRUMENT DAMAGE: Do not move the main interlock handle when you move the swing handle to the up position or you will open the interior ball valve, which might cause you to lose vacuum and possibly damage the instrument.

16. Remove the tool from the instrument.



Figure 8-15. Removing the Tool from the Instrument

17. Let the ion source cartridge cool.

- **A CAUTION** Hot Surface. Touching hot parts of the ion source interface might cause severe burns. During operation of the mass spectrometer, the ion source can reach temperatures up to 350 °C. Wait until the ion source has cooled down to room temperature before you begin working on it.
 - 18. Hold the handle of the source exchange tool with one hand and use the other hand to pull the barrel toward you and into the handle.



Figure 8-16. Exposing the Ion Source Cartridge

19. Invert the source exchange tool so that the barrel is pointed toward the floor.

20. Slide the source holder, which is in the MS toolkit, onto the end of the ion source cartridge. The opening of the source holder is designed to accommodate the handles of the ion volume.



Figure 8-17. Attaching the Source Holder

21. Twist the holder to disengage the ion source cartridge from the tool.

NOTICE The repeller locking nut is now loose on the repeller spring. Be careful not to tip the source or the components will fall out. ▲

22. Set the ion source cartridge and holder on a clean surface



Figure 8-18. Removing the Ion Source Cartridge

A CAUTION Hot Surface. The ion source parts might be hot, so use caution when handling.

- 23. Let the ion source cartridge cool down before removing it from the source holder.
- 24. Disassemble the ion source cartridge by removing the locking ring first, then the repeller spring, then the nut, insulator, and repeller (which comes out in one piece), ion volume, lens 1, lens 2, and lens 3/RF lens.

NOTICE IMPORTANT Many nitrile and latex gloves not certified for clean room use contain silicone mold releasing agents that will contaminate the instrument. For this reason, clean room gloves are strongly recommended when handling the ion source cartridge. We recommend Cardinal Health CP100 Nitrile Cleanroom Gloves. ▲



Figure 8-19. Components of the Q Exactive GC and Exactive GC Ion Source

- 25. Set the components on a clean work surface.
- 26. Replace the ion source cartridge or any individual component.

Reassembling the Ion Source Cartridge

* To reassemble the ion source cartridge.

1. Place the ion volume-repeller insulator on the repeller and hold it in place with the repeller nut. Set it aside for now.
2. Insert the ion cartridge sleeve into the source holder.



Figure 8-20. Inserting the Sleeve into the Source Holder

3. Align the long tooth of lens 3/RF lens with the notch on the bottom of the sleeve and drop the lens into the sleeve.



Figure 8-21. Inserting Lens 3/RF Lens into the Source Sleeve

4. Place lens 2 on top of lens 3/RF lens with the small hole facing down. It should fit snugly and sit evenly on top of lens 3/RF lens.



Figure 8-22. Inserting Lens 2 into the Source Sleeve

5. With the longer teeth of lens 1 facing down toward lens 2, align the larger metal section of lens 1 with the sleeve window and let it fall into place.



Figure 8-23. Inserting Lens 1 into the Source Sleeve

6. Insert the ion volume with the handles fitting into the notches of the sleeve. Make sure the ion volume is firmly seated into the gap on



lens 1. You may need to rotate lens 1 slightly to make the ion volume fit correctly.

Figure 8-24. Inserting the Ion Volume into the Source Sleeve

NOTICE The ion volume handles are different sizes and will only fit into the sleeve one way. ▲

- 7. Insert the ion volume repeller insulator onto the repeller.
- 8. Tighten the repeller nut.

9. Insert the large flat end of the repeller so that it rests on top of the ion volume.





10. Slide the repeller spring onto the repeller.



Figure 8-26. Inserting the Repeller Spring into the Sleeve

11. Place the locking ring on top of the repeller spring so that the repeller protrudes through the center hole on the locking ring. The hooks on the sleeve fit between the larger gaps on the locking ring.



Figure 8-27. Inserting the Locking Ring into the Sleeve



Reinserting the Ion Source Cartridge

NOTICE When inserting a cold ion source cartridge such as after cleaning or when switching between EI and CI modes, the ion source and lens stack will expand as the source cartridge heats, often pushing the ion volume and lenses away from the rear of the instrument where they are firmly held by the RF Lens spring contacts. To avoid intermittent electrical contacts to the lenses, you should insert the ion source cartridge, wait 30 minutes for it to get to temperature, then remove and reinsert it. ▲

* To reinsert the ion source cartridge

1. Hold the source holder and ion source cartridge in one hand and use the other hand to hold the ion cartridge tool so that the barrel is facing toward the floor. The diagram on the tool should be facing you. **NOTICE** If you try to attach the ion source cartridge to the tool by inverting it, the components will likely fall, so make sure you are working over a table. Otherwise, you may have to stop and clean the components again. ▲

2. Look for a small vertical 3mm line engraved on the end of the barrel. This line always matches up with the picture on the handle. There is a similar engraved line on the sleeve of the ion source cartridge. This line matches up with the filament.



Figure 8-28. Aligning the Tool with the Ion Source Cartridge

3. Position the engraved line on the tool with the open end of the hook on the sleeve. There is a pin the source exchange tool that will latch under the hook. 4. Push the ion source cartridge up into the barrel of the tool and twist it until the engraved lines are aligned. The ion source cartridge should easily slide into place with very little force.

NOTICE INSTRUMENT DAMAGE: If you push the ion source cartridge into the barrel and it will not slide easily into position, make sure the components are assembled correctly and have not slid out of place inside the sleeve. Using too much force when inserting the ion source cartridge into the barrel can cause damage. ▲

NOTICE The ion volume and lenses have keying features to assure the lens spring contacts will align with the metal parts of the lenses. ▲

5. Gently pull the source holder away from the ion source cartridge.



Figure 8-29. Removing the Source Holder

NOTICE When the source exchange tool is inverted, the source should stay attached. If this does not happen, the source will not insert correctly into the instrument. ▲

- 6. Turn the source exchange tool around so that the ion source cartridge is furthest away from you.
- 7. Firmly grasp the black handle of the ion cartridge tool in one hand and use your other hand to pull the metal barrel out and away from the handle so that tool is fully extended. The ion source cartridge is now hidden inside the barrel.

- 8. When the barrel can go no further, twist the handle to the left to lock it into position.
- 9. Insert the barrel end of the ion cartridge tool into the vacuum interlock and twist it to the right to lock it into position. Be sure the black handle remains in the locked position.



Figure 8-30. Evacuating the Instrument

- 10. Evacuate the VPI.
 - a. Confirm that the source removal tool is properly engaged in the VPI.
 - b. Press the blue **Evacuate** button on the front of the instrument.
 - c. The Evacuate light will begin to flash amber then green as the inlet evacuates, and should continue to flash green for approximately 20 seconds.
 - d. If the pressure has returned to an acceptable value after the 20-30 second wait, the evacuate light will turn off and the **Ready to Open** light will solid green. At that point, the air has been evacuated from the instrument and it is safe to open the vacuum interlock valve.
- 11. Pull the vacuum interlock handle up when the **Ready to Open** light is a solid green.
- 12. Twist the handle of the tool slightly to the left until it is feels like it is lodged into the left-most track.

NOTICE Make sure you take the correct track on the tool or the ion volume will disassemble inside the instrument. If that happens, the tool will get stuck and you will have to shut down, vent the instrument, and manually remove the source cartridge through the top of the instrument.



Figure 8-31. Pushing the Tool into the Instrument

13. Push the handle toward the instrument until the end of the handle aligns with the engraved line at the end of the barrel. When you reach this line, the tool is all the way in and the ion source cartridge has been placed back onto the ion source block. You may notice slight resistance when the handle is approximately 2 cm from the engraved line. This is normal. Do not force the cartridge into the instrument. To release the source from the spring contacts make small repeated rotations of the handle to the left and right quickly. Gently apply pressure to the back of the handle.

NOTICE Do not push down on the handle of the source exchange tool while inserting the ion source cartridge. This could result in opening an air leak that may cause your instrument to shut itself down to protect the vacuum pumps. ▲

NOTICE INSTRUMENT DAMAGE: Make sure the vacuum interlock handle is all the way up. Otherwise if you insert the tool with the handle down, you can damage the instrument. ▲

14. Twist the handle of the source exchange tool to the right and pull it back toward you and down the right side of the barrel's metal track until the line at the end of the track appears.



Figure 8-32. Pulling the Tool Down the Right Track

15. Pull the vacuum interlock handle down to close the interior ball valve.



Figure 8-33. Pulling Down the Vacuum Interlock Handle

16. Twist the end of the vacuum interlock handle and flip the swing handle up so that it rests next to the vacuum interlock knob location. Then twist the end again to hold it in place.

NOTICE INSTRUMENT DAMAGE: Make sure the vacuum interlock handle is all the way up. Otherwise if you insert the tool with the handle down, you can damage the instrument. Do not move the main interlock handle when you move the swing handle to the up position or you will open the interior ball valve, which might cause you to lose vacuum and possibly damage the instrument. ▲

- 17. Remove the tool from the instrument.
- 18. Reattach the vacuum interlock knob.

NOTICE Tip To prevent leaks in the vacuum interlock, we recommend that you leave the vacuum interlock knob attached to the instrument, except when you are removing or inserting the ion source cartridge. After you reattach the knob, press the **Evacuate** button will also eliminate any air inside the vacuum interlock. ▲

19. For optimal performance, wait at least 30 minutes for the ion source to heat up to the same temperature as the inside of the instrument. Otherwise, the masses or intensities may drift during operation.

Cleaning the Q Exactive GC or Exactive GC Ion Source Cartridge and Durable Components

NOTICE IMPORTANT If there is any doubt about a compatibility of decontamination of cleaning agents with parts of the equipment or material contained in it, the responsible party must contact Thermo Fisher Scientific product support personnel. ▲

You can ONLY clean the following durable components inside the vacuum manifold:

- Repeller
- Ion volume
- Lens 1
- Lens 2
- Lens 3/RF lens
- Ion cartridge sleeve
- Heat shield for the source interface board
- Screws

NOTICE You only need to clean the repeller, ion volume and all the lenses most frequently. Cleaning the other components are not part of the expected maintenance. ▲

To clean durable components of the Q Exactive GC or Exactive GC instrument, you will need the following cleaning supplies:

- Acetone, reagent grade (or other suitable polar solvent)
- Aluminum oxide abrasive powder, number 600
- Applicators, cotton-tipped
- Beaker
- Deionized water
- Detergent (Alconox, Micro, or equivalent)
- Dremel rotary tool or equivalent (recommended)
- Forceps
- Gas, clean and dry (Nitrogen, Helium or equivalent)
- Gloves, clean, lint- and powder-free, latex or nitrile
- Glycerol, reagent grade
- Toothbrush
- Cotton swab with wood handle
- Razor blade
- Ultrasonic cleaner

A CAUTION

Material and Eye Hazard. Wear impermeable laboratory gloves and eye protection when cleaning components.

- ***** To clean the durable components:
- 1. Remove contaminants from all the components you are cleaning.
 - a. Use a slurry of #600 aluminum oxide in glycerol on a cotton-tipped applicator to clean each component. Contamination can be indicated by a dark or discolored area, but it is often invisible. The heaviest contamination is usually found around the apertures, such as the electron entrance hole of the ion volume.

NOTICE Clean only the metal pieces of the repeller, lens 1 and lens 3/RF lens with aluminum oxide. ▲

 b. Clean each component thoroughly, even if no contamination is visible. To clean components faster, use a Dremel[™] tool and polishing swab at its lowest speed.

A WARNING Electric Current. Electric shock hazard. Exposing the Dremel tool to standing water may cause an electrical shock.

A WARNING Fire Hazard. Using the Dremel tool near flammable vapors may cause a fire.

- c. Clean the crevices of a component using a non-metal tool. It is very important to make sure you remove all of the debris or discoloration found in small edges of each component, in particular the ion volume. Otherwise, the debris or discoloration might affect the quality of your data.
- d. If you are cleaning the CI ion volume, use a razor blade to sharpen the wooden end of a wooden cotton swab to a 45° angle.

e. Twist the sharpened end of the swab into the electron entrance hole on the CI ion volume to clean out debris. You may need to use several swabs before the electron entrance hole is clear of debris.



Figure 8-34. Cleaning the Cl Ion Volume

NOTICE Tip Clean the CI ion volume under a microscope to verify that you removed all debris. ▲

- f. If you notice any deep scratches on the components, you may need to replace the component. Scratches can affect the performance of your instrument.
- 2. Rinse the components with clean tap water. Use a toothbrush under a stream of water to remove the aluminum oxide slurry. Do not let the slurry dry on the components because it is difficult to remove. If the components still look dirty, repeat step 1.
- 3. Sonicate the components in warm detergent.
 - a. Use forceps to place the components in a beaker of warm detergent.
 - b. Place the beaker and its contents in an ultrasonic bath for five minutes.
 - c. Rinse the components with tap water to remove the detergent.
- 4. Sonicate the components in deionized water.
 - a. Use forceps to place the components in a beaker of deionized water.

- b. Place the beaker and its contents in an ultrasonic bath for five minutes. If water is cloudy after sonicating, replace the water with fresh water, and put the beaker and contents in a ultrasonic bath again for five minutes. Repeat until the water is clear.
- 5. Use forceps to immediately transfer the components to a clean beaker of acetone.
- 6. Sonicate the components in acetone.

A WARNING Fire Hazard. Acetone is flammable and volatile, so make sure the ultrasonic bath is properly ventilated to prevent the buildup of vapors.

- a. Place the beaker and its contents in an ultrasonic bath for one minute.
- b. Use forceps to transfer the components to a beaker of fresh acetone.
- c. Place the beaker and its contents in an ultrasonic bath for one minute.
- 7. Wearing gloves, blow clean, dry gas on the components to remove the acetone.

Acetone should not be allowed to dry on the part. It will leave a residue that may affect instrument performance.

Refilling the Calibrant Reservoir of the Q Exactive GC or Exactive GC Mass Spectrometer

The calibrant reservoir should be refilled yearly or as needed.

- ✤ To refill the calibrant reservoir
- 1. Remove the small center panel in the front of the Q Exactive GC or Exactive GC mass spectrometer.



Figure 8-35. Opening the front panel

2. The calibration reservoir is located under the manifold. Twist the calibrant reservoir cover counter-clockwise and remove it from the calibration gas controller.



Figure 8-36. Locating the Calibrant Reservoir

3. Fill a syringe with 200 μ L of the FC 43 calibration compound, which contains perfluorotributylamine (PFTBA), and insert it into the calibrant reservoir.



Figure 8-37. Locating the Calibrant Reservoir

4. Inject the FC 43. If you see liquid pooled on top of the white frit, remove the excess liquid according to local environmental regulations.

NOTICE INSTRUMENT DAMAGE: Adding more than 300 μ L of calibration compound can damage the calibration gas controller. Be sure liquid does not get into the controller when you reattach the reservoir.

- 5. Reattach the cover to the calibration gas controller.
- 6. Reattach the front panel to the instrument.

Replacing a Dual Filament in the Q Exactive GC or Exactive GC Mass Spectrometer

The number of ions produced in the ion source is proportional to the filament emission current. If the measured emission current is substantially less than the set emission current value, or if the measured emission current is decreasing, you may need to replace the dual filament because it has failed or is failing. Also, if one of the filaments has burned out, it may be time to replace it.

You can increase the life of your dual filament by:

- Setting the solvent delay so that the analyzer will not turn on while the solvent peak is eluting.
- Not overriding the solvent delay at the beginning of a run.
- Selecting a lower emission current.

Click the Instrument Control button in the Xcalibur Status panel to switch between filaments A and B.

To replace a dual filament

1. Shut down the Q Exactive GC or Exactive GC system by following the steps in "Shutting Down the System" on page 6-7.

2. Use a T20 Torxhead screwdriver to remove the screws on the middle panel.



Figure 8-38. Locating the Screws on the Front Panel

3. Open the small center panel and remove the screw at the back of the panel using a flat-head screwdriver.





4. Carefully pull the entire central panel back to remove it. Set it aside.

5. Use a T20 Torxhead screwdriver to remove the four screws around the manifold door. The bottom two screws are behind the vacuum interlock panel.



Figure 8-40. Locating the Manifold Screws

6. Pull the manifold door out to open. Once the alignment pins are clear of the thumbscrews, swing the manifold door open.

7. Remove the glass manifold cover from the top of the manifold assembly.



Glass Manifold Cover

Figure 8-41. Locating the Glass Manifold Cover

NOTICE INSTRUMENT DAMAGE: Many nitrile and latex gloves not certified for clean room use contain silicone mold releasing agents that will contaminate the instrument. For this reason, clean room gloves are strongly recommended when touching components inside the vacuum manifold. We recommend Cardinal Health CP100 Nitrile Cleanroom Gloves. ▲

 Look through the top of the instrument and use a clean T10 Torxhead screwdriver to loosen the screw holding the filament retaining clip in place. Then rotate the clip away from the filament.



Figure 8-42. Loosening the Filament Retaining Clip Screw

- 9. Disconnect the filament board and wires from the source interface board.
- 10. Remove the filament.
- 11. Insert the replacement filament into its slot, rotate the spring into position, and slightly tighten the screw holding the filament retaining clip in place.
- 12. Bend the filament wires so they do not touch any metal component. You may want the old filament as a model.
- 13. Attach the connector of the replacement filament to the source interface board.
- 14. Return the glass manifold cover to the top of the instrument.
- 15. Swing the manifold door so that it is parallel to the opening. Guide the alignment pins into the thumbscrews.

NOTICE The manifold door will not swing closed. There will be a 1 cm gap. You must push the door to close it completely. Do not apply excess force to the thumbscrews or components may be damaged. \blacktriangle

NOTICE Once the manifold door is closed, ensure the filament wires do not contact the metal surface of the door. \blacktriangle

- 16. Use a T20 Torxhead screwdriver to replace the four screws around the manifold door. Do not overtighten the screws.
- 17. Reattach the front panel of the Q Exactive GC or Exactive GC.
- 18. Start up the instrument by following the steps in "Starting Up the System after a Shutdown" on page 6-9.

Maintaining GCs or Autosamplers

For instructions on maintaining GCs or autosamplers, refer to the manual that comes with the GC or autosampler.

Consumables

For information on consumables such as fittings, nitrogen gas, or cleaning agents, refer to the *Consumables* chapter in the *Q Exactive GC and Exactive GC Preinstallation Requirements Guide*.

The forepump oil is used for cooling, lubrication, and sealing of the forepump. See "Maintenance of the Forepump" on page 8-8 for information about forepump oil disposal. Also refer to the Material Safety Data Sheet (MSDS) for the forepump oil.

Thermo Fisher Scientific Service

This section contains information concerning maintenance work that must be performed by Thermo Fisher Scientific personnel.

Safety Advice for Possible Contamination

A CAUTION Hazardous Chemicals. Hazardous material might contaminate certain parts of your system during analysis. To protect our employees, we ask you to adhere to special precautions when returning parts to the factory for exchange or repair.

If hazardous materials have contaminated mass spectrometer parts, Thermo Fisher Scientific can only accept these parts for repair if they have been properly decontaminated.

Materials that due to their structure and the applied concentration might be toxic or which are reported in publications to be toxic are regarded as hazardous. Materials that will generate synergetic hazardous effects in combination with other materials present are also considered hazardous.

Parts contaminated by radioisotopes must not be returned to Thermo Fisher Scientific—neither under warranty nor within the exchange part program. If unsure about parts of the system possibly being contaminated by hazardous material, make sure the Thermo Fisher Scientific field service engineer is informed before the engineer starts working on the system.

Your signature on the Health and Safety Form confirms that the returned parts have been decontaminated and are free of hazardous materials. You can order the form from a Thermo Fisher Scientific field service engineer.

Services to be Performed by Thermo Fisher Scientific Service Only

Table 8-3 lists services that must be performed by a Thermo Fisher Scientific field service engineer only. Depending on the actual workload of your Q Exactive GC or Exactive GC mass spectrometer, you might increase the maintenance frequency.

| Fable 8-3. Thermo Fisher Scientific service procedures | | |
|---|-------------------------------------|-----------------------------|
| MS Component | Procedure | Frequency |
| Source TMP | Change operating fluid reservoir | Every three years |
| | Change TMP bearing | Every four years |
| Analyzer TMP | Change standard bearing | Every 45000 operating hours |

Chapter 9 Replaceable Parts

This chapter contains part numbers for replaceable and consumable parts for the mass spectrometer, data system, and kits. To ensure proper results in servicing the Q Exactive GC or Exactive GC system, order only the parts listed or their equivalent.

For information on how to order parts, see the contact information at the beginning of this manual.

Contents

- "Ion Source Components" on page 9-2
- "Filament Components" on page 9-2
- "Vacuum Interlock Components" on page 9-3
- "Tools" on page 9-4
- "Pump Components" on page 9-4
- "Calibration Gas Components" on page 9-5
- "Analyzer Components" on page 9-5
- "Source Electronics Components" on page 9-5
- "Consumables" on page 9-6
- "Other Parts" on page 9-6

Ion Source Components

| EI Ion Source Cartridge (Low Activity), includes below: . 1R120404-4100 |
|---|
| Ion Cartridge Sleeve 1R120404-1105 |
| EI Ion Volume (Low Activity) |
| Ion Volume-Repeller Insulator 1R120404-1114 |
| Repeller (Low Activity) |
| Ion Volume Locking Ring 1R120404-1118 |
| Repeller Spring (pkg of 5) |
| Repeller Nut |
| Lens 3/RF Lens |
| Lens 1 |
| Lens 2 1R120404-1140 |
| CI Reagent Gas Flow Module 1R123331-0092 |
| CI Ion Volume |
| CI Ion Source Cartridge Assembly |
| EI/CI Ion Volume |
| Spring Contact Assembly 1R120404-1750 |

Filament Components

| Dual Filament | 1R120404-1940 |
|-------------------------------------|---------------|
| Filament Retaining Spring Kit | 1R120404-1405 |
| Screw for Filament Retaining Spring | 1R76913-0305 |

Vacuum Interlock Components

| nner Ball Seal1R120406-1008 | 8 |
|--|---|
| /alve Axle1R120406-1003 | 3 |
| 1R120406-2204 | 4 |
| xle Bearing1R120406-1005 | 5 |
| ealing Ball1R120406-1004 | 4 |
| Duter Ball Seal | 2 |
| Handle1R120406-1200 | 0 |
| /alve1R76461-5002 | 2 |
| /alve Spring (Pkg of 5) 1R76485-1000k | ζ |
| /acuum Interlock Knob1R120406-3000 | 0 |
| Vacuum Interlock Assembly | 1 |
| Tubing (cm) | 7 |
| Barb Fitting—"L"1R76256-1332 | 2 |
| Barb Fitting—Straight | 0 |
| Vacuum Interlock Microswitch Assembly1R120406-1030 | 0 |
| nterior O-ring1R3814-127 | 7 |
| Exterior O-ring1R3815-320 | 0 |
| Clip (Pkg of 5) | 2 |
| | |





Tools

| Bushing in the Source Exchange Tool 1R120406-2203 |
|--|
| Seal in the Source Exchange Tool 1R120406-2204 |
| Clip in the Source Exchange Tool |
| Source Exchange Tool 1R120406-2000 |
| VPI Toolkit, which includes*: |
| Source Holder |
| Source Removal Tool (Small) |
| Source Plug |
| Source Plug Holder |
| CI Ion Volume |
| EI/CI Ion Volume |
| T10 Torxhead Key1R3812-5T10 |
| T20 Torxhead Key1R3812-5T20 |
| T30 Torxhead Key1R3812-5T30 |
| Forceps, 8 in |
| Wrench, Open-Ended, 1/4-in., 5/16-in |
| Wrench, Open-Ended, 3/8 in., 7/16-in 1R76360-0108 |
| Wrench, Open-Ended, 1/2-in., 9/16-in 1R76360-0110 |
| Wrench, Open-Ended, 1/2 in., 7/16-in 1R76360-0111 |
| *The VPI tool kit also includes the Source Exchange Tool (P/N 1R120406-2000) |

Pump Components

| 1R76505-3007 |
|--------------|
| 1R76505-5003 |
| 1R76505-2002 |
| 1R76505-2001 |
| 1R76505-0036 |
| 1R76505-5002 |
| A0301-15101 |
| |

Calibration Gas Components

| Dual Flow Calibration Gas Module | 1R119246-0003 |
|----------------------------------|---------------|
| Calibrant Reservoir Kit | 1R120433-0001 |
| MS Transfer Line | 1R120705-0016 |
| GC Transfer Line | 1R120705-0017 |
| | |

Analyzer Components

| 1R120610-0020 |
|---------------|
| 1R120705-0020 |
| 1R120705-0003 |
| 1R120705-0102 |
| 1R120705-0030 |
| 1R120705-0148 |
| |

Source Electronics Components

| Electronics Box Assembly | 1R120705-0023 |
|--|--------------------------|
| Lens Interface Board | 1R120578-0210 |
| IOS RF Board | 1R120705-0060 |
| Source Board (Exactive GC only) | 1R120578-0300 |
| Translator Board | 1R120578-0010 |
| Controller Interface Board | 1R120578-0020 |
| Distribution Board | 1R120578-0810 |
| Lens Driver Board | 1R120578-A110 |
| Power Supply for Boards (250 W AC/DC, 24 V | 7, 10.4 A) .1R76330-0250 |

Consumables

| Transfer Line Nut Kit (High Temp) | .1R120434-0100 |
|--|-----------------|
| Custom Vespel High-temperature Ferrule (Pkg of 5) | 290VT221 |
| Spring-loaded Transfer Line Nut | . 1R120434-0020 |
| Long Graphite/Vespel ferrule 0.1–0.25 mm i.d. (Pkg of 10) | 29033496 |
| Short Graphite/Vespel ferrule 0.1–0.25 mm i.d. (Pkg of 10) | 290VA191 |
| Transfer Line Seal Kit | . 1R120705-0204 |
| Mixing Chamber Bushing | . 1R120705-0141 |
| Ion Source Insulators | . 1R120705-0090 |
| Performance Kit (Test Standards) | 1R120705-PERF |
| Brass Transfer Line Nut (Use with long G/V ferrule) | 1R76256-0060 |
| Calibration Compound | . 1R50010-30059 |

Other Parts

Gas Supply Parts

Ethernet Switch and Cables

| Switch | |
|----------------------------|--|
| Patch cord, RJ45 SFTP, 5 m | |
| Patch cord, RJ45 SFTP, 1m | |

Additional Power Components

| Power cord; 16A/230V, C19, 5M UL | 2112490 |
|----------------------------------|---------|
| Power strip | 2129880 |

Fan Filter

Aux Temperature Module

| Aux Temperature | Module | | 19070080 |
|-----------------|--------|--|----------|
|-----------------|--------|--|----------|

CI Gas Module

| CI Gas Module | | . 1R23331-0092 |
|---------------|------|--------------------|
| | | |

Q Exactive GC Series Probe Kit

| Probe Kit | R120705-0036 |
|-----------|--------------|
|-----------|--------------|

Legal Documents

Contents

- "FCC Compliance Statement" on page D-2
- "WEEE Compliance" on page D-3
- "Declaration of Conformity for Q Exactive GC MS" on page D-4
- "Declaration of Conformity for Exactive GC MS" on page D-5

FCC Compliance Statement

THIS DEVICE COMPLIES WITH FCC PART 15 SUBPART B AND INDUSTRY CANADA: ICES-003 ISSUE 5, AUGUST 2012 FOR A CLASS A DEVICE.
WEEE Compliance

This product is required to comply with the European Union's Waste Electrical & Electronic Equipment (WEEE) Directive 2012/19/EU. It is marked with the following symbol:



Thermo Fisher Scientific is registered with B2B Compliance (B2Bcompliance.org.uk) in the UK and with the European Recycling Platform (ERP-recycling.org) in all other countries of the European Union and in Norway.

If this product is located in Europe and you want to participate in the Thermo Fisher Scientific Business-to-Business (B2B) Recycling Program, send an email request to weee.recycle@thermofisher.com with the following information:

- WEEE product class
- Name of the manufacturer or distributor (where you purchased the product)
- Number of product pieces, and the estimated total weight and volume
- Pick-up address and contact person (include contact information)
- Appropriate pick-up time
- Declaration of decontamination, stating that all hazardous fluids or material have been removed from the product

NOTICE This recycling program is not for biological hazard products or for products that have been medically contaminated. You must treat these types of products as biohazard waste and dispose of them in accordance with your local regulations. ▲

RoHS

For information about the Restriction on Hazardous Substances (RoHS) Directive for the European Union, search for RoHS on the Thermo Fisher Scientific European language websites.

Declaration of Conformity for Q Exactive GC MS

-Original-

EG-Konformitätserklärung *EC Declaration of Conformity*

CE



Thermo Fisher Scientific (Bremen) GmbH Hanna-Kunath-Str. 11 28199 Bremen, Germany

Wir erklären hiermit, dass das folgende Produkt *We hereby declare that the following product*

Bezeichnung: Designation: Massenspektrometer Mass Spectrometer

Modell: Model: **Thermo Scientific Q Exactive GC Orbitrap** *Thermo Scientific Q Exactive GC Orbitrap*

alle einschlägigen Anforderungen der folgenden Richtlinien erfüllt: fulfills all the relevant requirements of the following directives:

Niederspannungsrichtlinie Low Voltage Directive Richtlinie über elektromagnetische Verträglichkeit Electromagnetic Compatibility Directive

2014/35/EU 2014/35/EU **2014/30/EU** 2014/30/EU

Die folgenden einschlägigen harmonisierten Normen wurden zugrunde gelegt: *The following relevant harmonized standards were used:*

EN 61010-1:2010 EN 61010-1:2010 EN 61326-1:2013 EN 61326-1:2013

Für die Zusammenstellung der technischen Unterlagen ist bevollmächtigt: *Person authorized to compile the technical file:*

Jörg Behrens (Director Operations) Thermo Fisher Scientific (Bremen) GmbH

27 Unterschrift Signature

Bremen, 2016-04-18

Datum Date

Declaration of Conformity for Exactive GC MS

-Original-

CE

EG-Konformitätserklärung *EC Declaration of Conformity*



Thermo Fisher Scientific (Bremen) GmbH Hanna-Kunath-Str. 11 28199 Bremen, Germany

Wir erklären hiermit, dass das folgende Produkt *We hereby declare that the following product*

Bezeichnung: Designation: Massenspektrometer Mass Spectrometer

Modell: Model: **Thermo Scientific Exactive GC** *Thermo Scientific Exactive GC*

alle einschlägigen Anforderungen der folgenden Richtlinien erfüllt: fulfills all the relevant requirements of the following directives:

Niederspannungsrichtlinie Low Voltage Directive Richtlinie über elektromagnetische Verträglichkeit Electromagnetic Compatibility Directive

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D DC Unterschrift Signature

Bremen, 2016-04-18

Datum Date

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