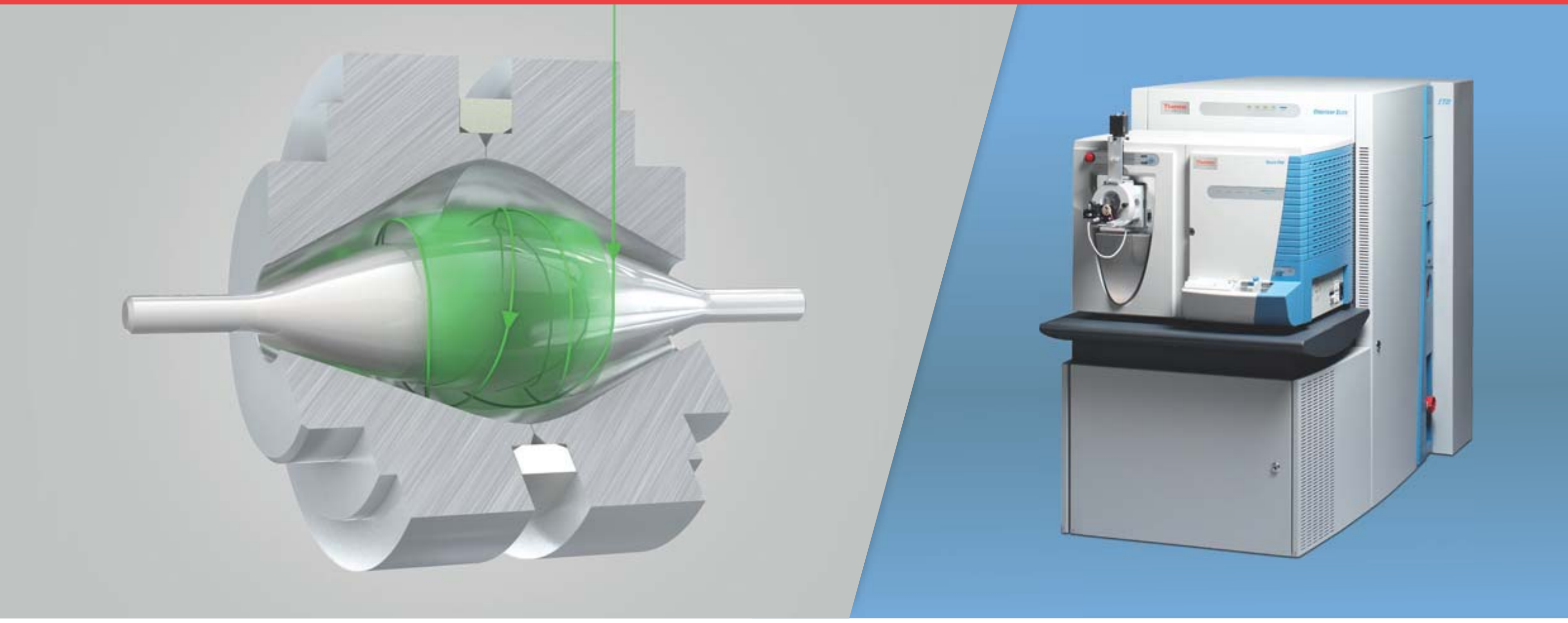

Orbitrap Elite

Operating Manual

1288171 Revision B July 2017

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Original Operating Instructions

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Contents

Technical Data for Orbitrap Elite Systems

The table summarizes the most important technical data of the Orbitrap Elite systems. See the respective chapters of the manual for details and additional instrument properties.

Table 1-1. Technical Data for Orbitrap Elite Systems

Parameter	Specification		Value
Instrument Properties			
Mass Spectrometer	Length × width × height Weight		1463 × 870 × 1414 mm (1705 × 913 × 1414 mm)[a] 685 kg (810 kg)[a]
Recirculating Chiller	Length × width × height Weight		624 × 360 × 692 mm 59.2 kg
Complete System (incl. data system and recirculating chiller)	Heat generation		5.5 kW (6.2 kW)[a]
Power Requirements			
Mass Spectrometer	Input	Nominal voltage Fuse[b]	230 V AC, 50/60 Hz, three phases 3×16 A (tripping characteristic B)
	Output	1×	230 V AC, 50/60 Hz, max. 16 A
Recirculating Chiller	Input	Nominal voltage Fuse[b]	115 V AC, 60 Hz / 230 V AC, 50 Hz 15/16 A
Data System[c]	Input	Nominal voltage Fuse[b]	200–240 V AC, 50/60 Hz 15/16 A
Gas Requirements			
Helium	Purity		99.999% or better (ultra-high purity), less than 1 ppm each of water, oxygen, and total hydrocarbons
	Pressure		275 ± 70 kPa
Nitrogen	Purity		99% or better (high purity)
	Pressure		690 ± 140 kPa
ETD Reagent Carrier Gas[d]	Purity		99.999% or better (ultra high purity), less than 3 ppm each of water, oxygen, and total hydrocarbons
	Pressure		690 ± 140 kPa
Operating Environment			
	Laboratory temperature Max. temperature fluctuation Humidity		15–27 °C 5 °C/5 min 50–80%, non-condensing and non-corrosive atmosphere
Exhaust Requirements	Inrush flow rate Continuous flow rate		3 L/min 1 L/min

[a] In case of an Orbitrap Elite ETD MS.

[b] Dedicated wall outlet.

[c] The Orbitrap Elite MS provides electric power for the data system. The Orbitrap Elite ETD MS provides electric power for the ETD Module and the data system is connected to a wall outlet.

[d] Thermo Fisher Scientific strongly recommends a mixture of 25% helium and 75% nitrogen. If the helium/nitrogen mixture is not available, then use nitrogen.

Chapter 1 Using this Manual

Welcome to the Thermo Scientific Orbitrap Elite system! The Orbitrap Elite mass spectrometer is a member of the family of LTQ™ mass spectrometer (MS) hybrid instruments.

All information in this manual concerning the Orbitrap Elite mass spectrometer also applies to the Orbitrap Elite ETD system where the ETD Module is physically coupled to the back of the Orbitrap Elite mass spectrometer.

Contents

About this Manual

This *Orbitrap Elite 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 Orbitrap Elite instrument. In addition, this manual provides step-by-step instructions for cleaning and maintaining your instrument.

Typographical Conventions

This section describes typographical conventions that have been established for Thermo Fisher Scientific manuals.

Signal Word

Make sure 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 *left* and *right* 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 via 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>**" means press the key labeled *F1*.
- Any command that requires pressing two or more keys simultaneously is shown with a plus sign connecting the keys. For example, "press **<Shift>** + **<F1>**" means press and hold the <Shift> key and then press the <F1> key.
- 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 *Orbitrap Elite Operating Manual* represents the Original Operating Instructions. In addition to this manual, Thermo Fisher Scientific provides other documents for the Orbitrap Elite mass spectrometer that are not part of the Original Operating Instructions. Reference documentation for the Orbitrap Elite mass spectrometer includes the following:

- *LTQ Orbitrap Series Preinstallation Requirements Guide*
- *Orbitrap Elite Getting Started*
- Velos Pro manual set

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**

1. From the Microsoft™ Windows™ taskbar, choose **Start > Programs > Thermo Instruments > LTQ > Manuals > *model***.
2. Click the PDF file that you want to view.

A printed version of this *Orbitrap Elite Operating Manual* is shipped with the instrument. A printed version of the *LTQ Orbitrap Series Preinstallation Requirements Guide* is part of the Preinstallation Kit. This kit is sent to your laboratory before the arrival of the Orbitrap Elite mass spectrometer.

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

- Forepumps
- Turbomolecular pumps
- Data system computer and monitor
- Recirculating chiller
- Safety data sheets

Contacting Us

There are several ways to contact Thermo Fisher Scientific.

Assistance

❖ **To get brochures and ordering information**

Web site	www.thermofisher.com/orbitrap

❖ **To contact Customer Service**

Web site	www.unitylabservices.com

❖ **To get user manuals for your product**

Customer SharePoint	www.thermoscientific.com/Technicaldocumentation

1. With the serial number (S/N) of your instrument, request access on our customer SharePoint as a **customer**.

   For the first login, you have to create an account. Follow the instructions given on screen. Accept the invitation within six days and log in with your created Microsoft™ password.

2. Download current revisions of user manuals and other customer-oriented documents for your product. Translations into other languages may be available there as well.

Suggestions to the Manual

❖ **To suggest changes to this manual**

- Send your comments to:

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

- Send an e-mail message to the Technical Editors at

  documentation.bremen@thermofisher.com

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

Chapter 2 Functional Description

This chapter provides an overview of the functional elements of the Orbitrap Elite mass spectrometer.

Contents

General Description

The Orbitrap Elite mass spectrometer is a hybrid mass spectrometer incorporating the Velos Pro™ dual cell linear trap and the high-field Orbitrap™ analyzer. Figure 2-1 shows a front view of the instrument.

Figure 2-1. Orbitrap Elite MS front view

The Orbitrap Elite mass spectrometer consists of four main components (See Figure 2-2 on page 2-3.), which are described in the following topics:

- Dual cell linear ion trap (Thermo Scientific Velos Pro MS) for sample ionization, precursor ion selection, fragmentation, and AGC™.
- Intermediate storage device (curved linear trap) that is required for short pulse injection.
- High-field Orbitrap analyzer for Fourier transformation based analysis.
- Collision cell for performing higher energy CID experiments.

The Orbitrap Elite ETD mass spectrometer has an additional reagent ion source for performing Electron Transfer Dissociation (ETD) experiments. See “ETD System” on page 2-19.

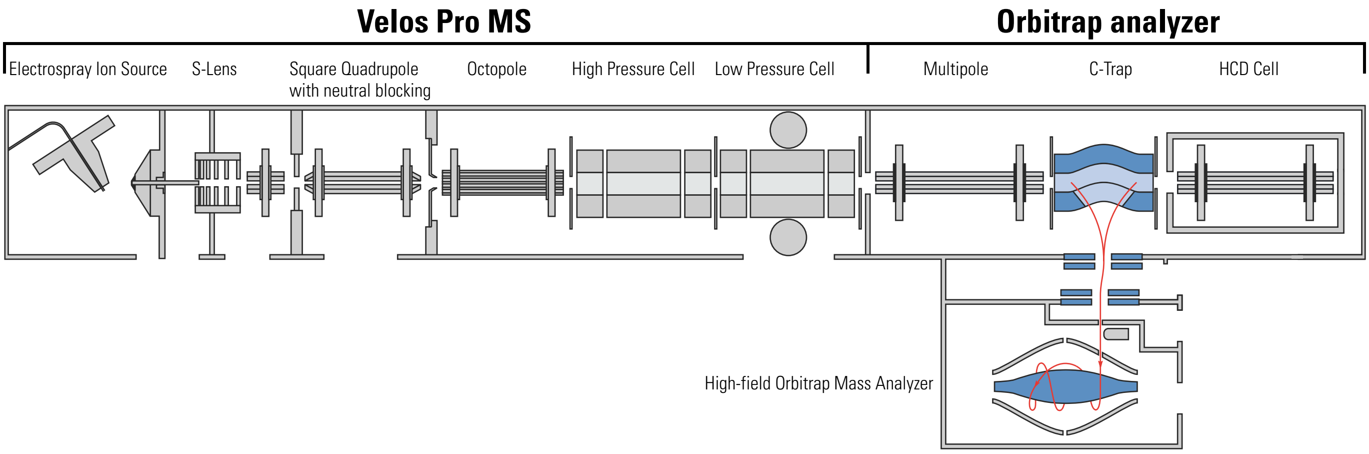


Figure 2-2. Schematic of the Orbitrap Elite MS

Mechanical Characteristics

Wheels at the bottom side of the instrument facilitate positioning the Orbitrap Elite mass spectrometer at the intended place in the laboratory.

The mains inlet as well as a power outlet for peripheral devices are at the right side of the instrument. The forepumps for the vacuum system of the linear trap and the Orbitrap analyzer are hidden under the linear trap and accessible from the front. The forepump for the ETD Module is accessible after removing the bottom panel of the rear side. The left side panel and the front panel of the MS portion are mounted on hinges and the right side panel is removable. The top lid of the MS portion opens upwards to allow easy access for Thermo Fisher Scientific field service engineers from the top. See Figure 2-3.

Figure 2-3. Top lid of MS portion opened

In the Orbitrap Elite ETD mass spectrometer, after removing the cables, the top lid of the ETD Module is also removable to allow accessing its electronic components.

A stand-alone recirculating water chiller is shipped with the instrument. It is connected to the right side of the instrument.

Specifications

The Orbitrap Elite mass spectrometer has the following measuring specifications:

Resolution	60000 (FWHM) at *m/z* 400 at a scan rate of 4 Hz, minimum resolution 15000 (FWHM) maximum resolution > 240000 (FWHM) at *m/z* 400
Cycle Time	> 4 scans at 60000 (FWHM) resolution @ *m/z* 400 per second
Mass Range	*m/z* 50–2000; *m/z* 200–4000
Mass Accuracy	<3 ppm RMS for 2 h period with external calibration using defined conditions, <1 ppm RMS with internal calibration
Dynamic Range	>10000 between mass spectra, >5000 between highest and lowest detectable ion signal in one spectrum
MS/MS	MS/MS and MS^n scan functions

Control Elements

The Orbitrap Elite mass spectrometer is mainly operated from the desktop computer (data system). Some control elements for important system functions are directly on the instrument. They are described in the following sections.

System Status LEDs

Figure 2-4 shows the system status LEDs at the front of the instrument. Five LEDs indicate the main functions of the system. (See also Figure 2-5 on page 2-6.) The Power LED is directly controlled by the 3 × 230 V input and all other LEDs are controlled by the power distribution board (See "Power Distribution Board" on page 2-52). Table 2-1 explains the function of the various LEDs.

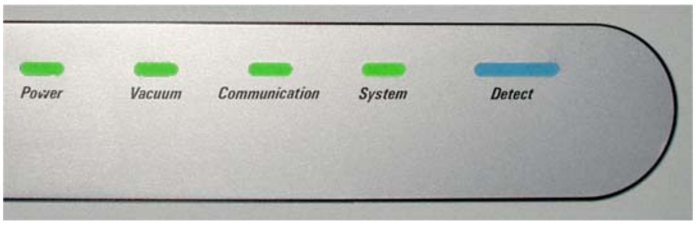


Figure 2-4. System status LEDs

The system status LEDs at the front panel of the linear ion trap are described in the *LTQ Series Hardware Manual*.

Table 2-1. System status LEDs of the Orbitrap Elite MS

LED	Status	Information
Power	Green Off	Main switch on Main switch off
Vacuum[a]	Green Yellow	Operating vacuum reached Insufficient vacuum or Vacuum Pumps switch off
Communication	Green Yellow	Communication link between instrument and data system established Communication link starting up or Vacuum Pumps switch off
System[a]	Green Yellow	System ready FT Electronics switch off or Vacuum Pumps switch off
Detect	Blue Off	Orbitrap analyzer is scanning Orbitrap analyzer is not scanning

[a] These LEDs are flashing when a system bakeout is performed. See "Baking Out the System" on page 6-6.

Control Panels

Figure 2-5 shows the right side of the Orbitrap Elite mass spectrometer. Here are the control panels, switches, and the ports for the external connections (mains supply, gases, Ethernet communication, and cooling water).

Figure 2-5. Right side of the Orbitrap Elite MS

For more information about the external connections, see "External Connections" on page 2-9.

Upper Control Panel

The upper instrument control panel comprises the bakeout timer, the bakeout control buttons, and three circuit breakers. To access the upper control panel, swing open the small lid (opens from left to right). See Figure 2-5 and Figure 2-6 on page 2-7.

Use the timer to set the duration for the bakeout of the system. After the duration is set, press the green button on the right to start the bakeout procedure. To stop a running bakeout procedure, press the orange button on the left side. For instructions about performing a bakeout, see "Baking Out the System" on page 6-6.

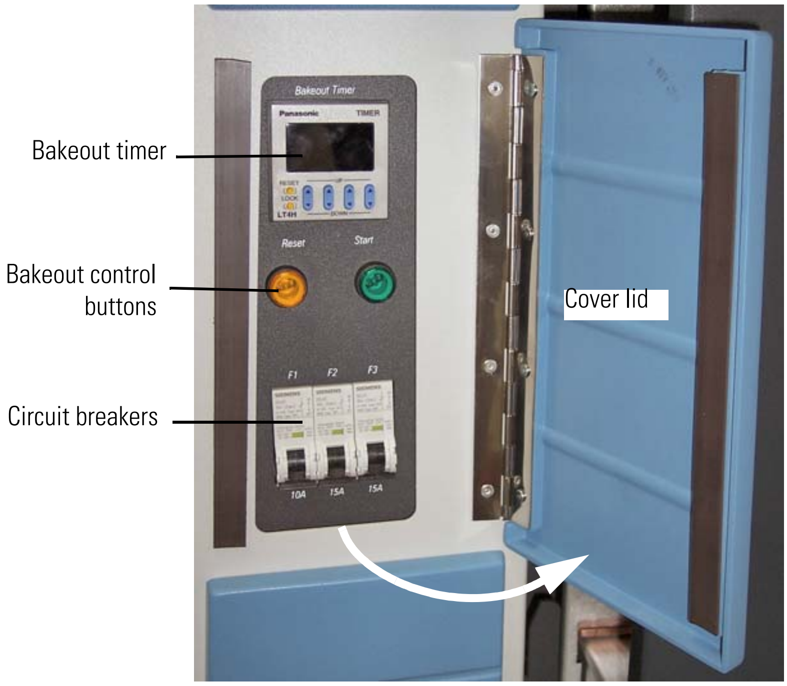


Figure 2-6. Upper control panel

NOTICE The buttons themselves have no indicator function. A running bakeout procedure is indicated by the flashing Vacuum LED and System LED at the front side of the instrument. See Figure 2-4 on page 2-5. ▲

Three circuit breakers are at the bottom of this control panel. Table 2-2 shows the parts of the Orbitrap Elite mass spectrometer that are protected by the respective circuit breaker. The proper function of each circuit breaker is signaled by a dedicated LED in the power control panel (for example, F1 corresponds to L1).

Table 2-2. Circuit breakers of the Orbitrap Elite MS

Circuit breaker	Ampere	LED	Instrument parts
F1	10	L1	Power Distribution
F2	15	L2	Linear ion trap
F3	15	L3	Multiple socket outlets (Peripherals, LC, heater, etc.)

Power Control Panel

In addition to the system status LEDs at the front side (see Figure 2-4 on page 2-5), the Orbitrap Elite mass spectrometer has three power control LEDs above the Vacuum Pumps switch at the right side. See

Figure 2-7. They indicate whether the corresponding circuit breaker is closed and the respective parts of the instrument have power. (See Table 2-2.)

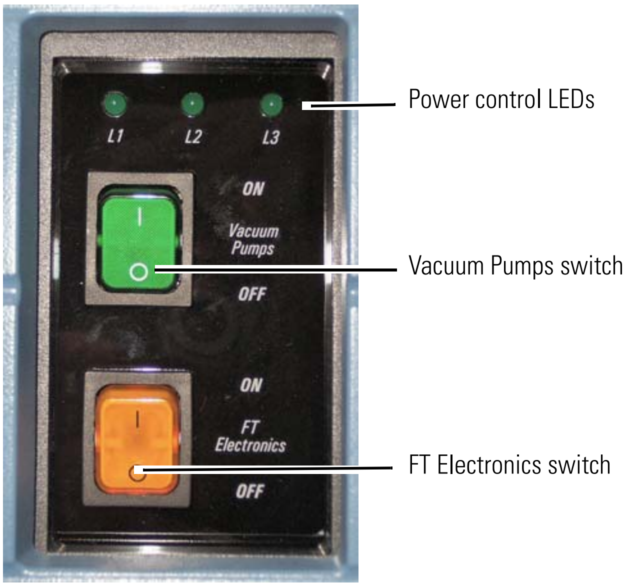


Figure 2-7. Power control panel with power control LEDs and switches

The use of the switches below the power control LEDs changes the working mode of the power distribution. (See "Working Modes of the Power Distribution" on page 1-48.)

The Vacuum Pumps switch can be set into the positions **ON** or **OFF**. When the switch is in the **OFF** position, everything but the multiple socket outlet is switched off.

The FT Electronics switch can be set into the operating position (**ON**) or into the service position (**OFF**). When the switch is in the service position, all components are switched off with exception of the following:

- Fans
- Heater control
- Power distribution (See "Power Distribution Board" on page 2-52)
- Pumps (See "Vacuum System" on page 2-30)
- Temperature controller (See "Temperature Controller Board" on page 2-60)
- Vacuum control

The linear ion trap also remains on because it has a separate Service switch.

Main Power Switch

The main power switch must be turned 90° clockwise/counterclockwise to switch on/off the instrument (see Figure 2-8). Placing the main power switch in the Off position switches off all power to the Orbitrap Elite mass spectrometer, the linear ion trap, and the vacuum pumps. In the Orbitrap Elite ETD mass spectrometer, power to the ETD Module is also switched off.

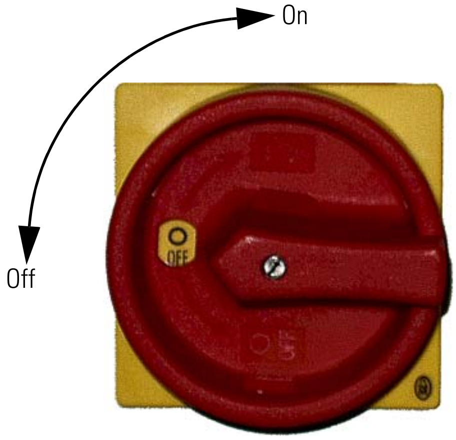


Figure 2-8. Main power switch

NOTICE When the main power switch is in the Off position, you can secure it with a padlock or a cable tie (to prevent unintended re-powering when performing maintenance, for example). ▲

External Connections

Figure 2-9 shows the lower right side of the instrument with the external connections for mains supply, gases, cooling water, and Ethernet communication.

At the top are two ports for Ethernet cables for connecting the Orbitrap Elite mass spectrometer and the linear ion trap via an Ethernet hub with the data system computer.

The power outlet for peripheral devices is below the Ethernet ports. In the Orbitrap Elite MS, the outlet provides the mains supply for the data system. In the Orbitrap Elite ETD MS, the outlet provides the mains supply for the ETD Module whereas the data system is connected to a wall outlet.

The power connector for the mains supply is at the center. The Orbitrap Elite MS is 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.

NOTICE Systems installed in areas with 208 V power experience voltage sags during high use periods that might place the line voltage below the operating parameters discussed in this section. In this case, you must protect your instrument by using a buck/boost transformer to ensure that power is within the specified parameters at all times. ▲

Figure 2-9. External connections to the Orbitrap Elite MS

The cooling water ports are below the power connector. (See also "Cooling Water Circuit" on page 2-41.)

The port for nitrogen gas allows connecting a Teflon™ hose from the gas supply of the laboratory to the instrument. The required gas pressure for nitrogen is 690 ± 140 kPa (6.9 ± 1.4 bar, 100 ± 20 psi). Helium (40 ±10 psi [275 ±70 kPa], 99.999% [ultra-high] purity) enters the instrument through a 1/8 inch port. Metal tubing from the helium gas supply must be terminated with 1/8 inch, female, Swagelok-type connectors. See "Gas Supply" on page 4-5 for information about connecting the gas supplies to the instrument.

[1] The port named Collision Gas is not used in the Orbitrap Elite MS.

NOTICE Do not connect other gases than nitrogen or helium to the Orbitrap Elite mass spectrometer! The maximum pressure for the nitrogen gas inlet is 830 kPa (8.3 bar, 120 psi); the maximum pressure for the helium inlet is 345 kPa (3.45 bar, 50 psi). ▲

In the Orbitrap Elite ETD mass spectrometer, the ETD reagent carrier gas supply of the laboratory is connected via metal tubing to an1/8 inch inlet port at the rear side of the instrument. Metal tubing from the gas supply must be terminated with 1/8 inch, female, Swagelok-type connectors. The required gas pressure is 690 ± 140 kPa (6.9 ± 1.4 bar, 100 ± 20 psi). See “Gas Supply of the Reagent Ion Source” on page 2-39.

The exhaust hose from the rotary pumps comes out of the back of the instrument, and connects the pumps to the exhaust system in the laboratory.

Linear Ion Trap

The Orbitrap Elite system can use a variety of ionization techniques such as ESI, APCI, or APPI. Maintenance of the Ion Max API source, as well as switching between ionization methods, is vent-free. Ions are transferred by octapole and "square" quadrupole lenses into an ion trap that is optimized for axial ion ejection into the curved linear trap. (See Figure 2-2 on page 2-3.)

The linear ion trap is an independent MS detector (Thermo Scientific Velos Pro), which can store, isolate, and fragment ions and then send them either to the Orbitrap analyzer for further analysis or to an SEM detector. The linear ion trap is a unique ion preparation and injection system for Orbitrap MS, because it has greater ion storage capacity than conventional 3D ion trap devices. The linear ion trap is described in the *LTQ Series Hardware Manual*.

All the ion handling, selection and excitation capabilities of the ion trap can be used to prepare ions for analysis in the Orbitrap analyzer. These features include storage and ejection of all ions, storage of selected *m/z* ranges, as well as ion isolation. Isolated ions can be excited and then fragmented as necessary for MS/MS and MS^n experiments. The patented Automatic Gain Control (AGC) provides extended dynamic range and insures optimized overall performance of the ion trap and Orbitrap MS.

The application of a supplementary RF voltage on the end lenses of the linear trap allows ions of opposite polarity to be trapped in the same space at the same time (charge-sign independent trapping—CSIT). This allows performing ion-ion reactions of previously isolated precursor cations with ETD reagent anions.

The linear ion trap and the transfer chamber are mounted on a table. See Figure 2-1 on page 2-2. The table also serves as a housing for the forepumps. See Figure 2-25 on page 2-33. The Orbitrap Elite mass spectrometer provides power for the linear ion trap. The Orbitrap Elite ETD mass spectrometer also provides the power for the ETD Module.

The linear ion trap is delivered with power connector, gas lines (He, N_2), and vacuum tube lines extending to the ESI source. On the rear side of the Velos Pro ion trap is a flange with an O-ring seal. When the flange is removed, the Orbitrap transfer chamber is mounted to the flange of the linear ion trap. The transfer chamber is held with supports on the table. The components of the ion optics and the Orbitrap analyzer are fixed to the transfer chamber.

Curved Linear Trap

On their way from the linear trap to the Orbitrap analyzer, ions move through the gas-free RF-only octapole into the gas-filled curved linear trap (C-Trap). See Figure 2-10. Ions entering the C-Trap loose their kinetic energy in collisions with nitrogen bath gas emanating from the HCD cell 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 to cool them down to the axis of the C-Trap.

Voltages on the end apertures of the curved 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 smaller package along this axis. The RF to the C-Trap (“Main RF”) is provided by the CLT RF main board. (See page 2-62.) Entrance and exit DC voltages as well as RF voltages to the transfer multipole are all provided by the ion optic supply board. (See page 2-58.) High voltages to the lenses are provided by the high voltage power supply board. (See page 2-64.)

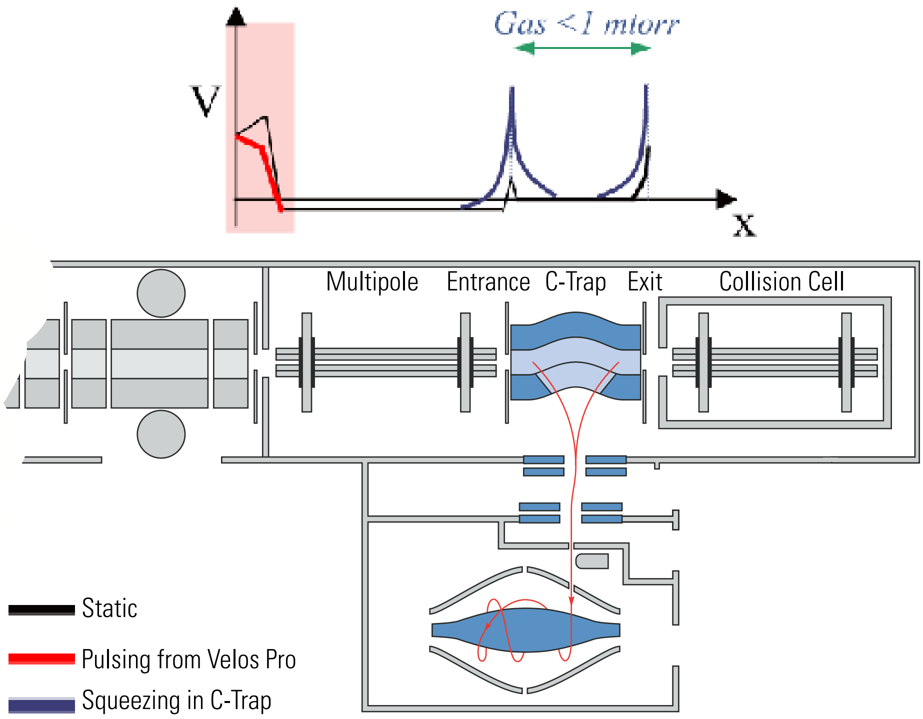


Figure 2-10. Layout of the Orbitrap Elite MS, also showing the applied voltages

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 2-11. The Orbitrap analyzer employs electric fields to capture and confine ions.

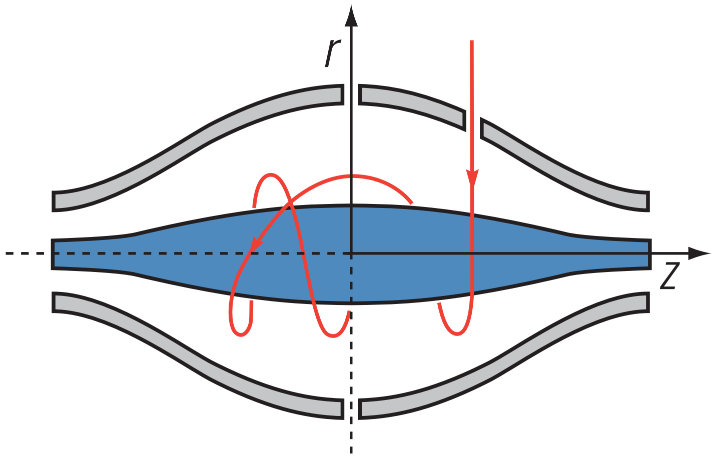


Figure 2-11. Schematic of Orbitrap cell and example of stable ion trajectory

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) form also 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 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/charge. Such durations are considerably shorter than a half-period of axial ion oscillation in the trap. When ions are injected into the Orbitrap analyzer at a position offset from its equator (See Figure 2-12.), these packets start coherent axial oscillations without the need for any additional excitation cycle.

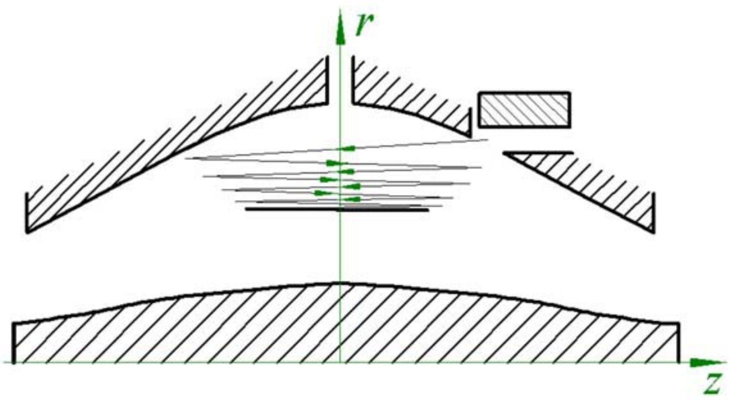


Figure 2-12. Principle of electrodynamic squeezing of ions in the Orbitrap analyzer as the field strength is increased

The evolution of an ion packet during the increase of the electric field is shown schematically on Figure 2-12. 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.

Measuring Principle

In the mass analyzer shown in Figure 2-11 on page 2-14, stable ion trajectories combine rotation around an axial central electrode with harmonic oscillations along it. The frequency ω of these harmonic oscillations along the z-axis depends only on the ions' mass-to-charge ratios *m/z* and the instrumental constant *k*:

$$w = \sqrt{\frac{z}{m} \times k}$$

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 2-12 on page 2-15.), 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 of half of the outer electrode is differentially amplified and then undergoes analog-to-digital conversion before processing using the Fourier transform algorithm.

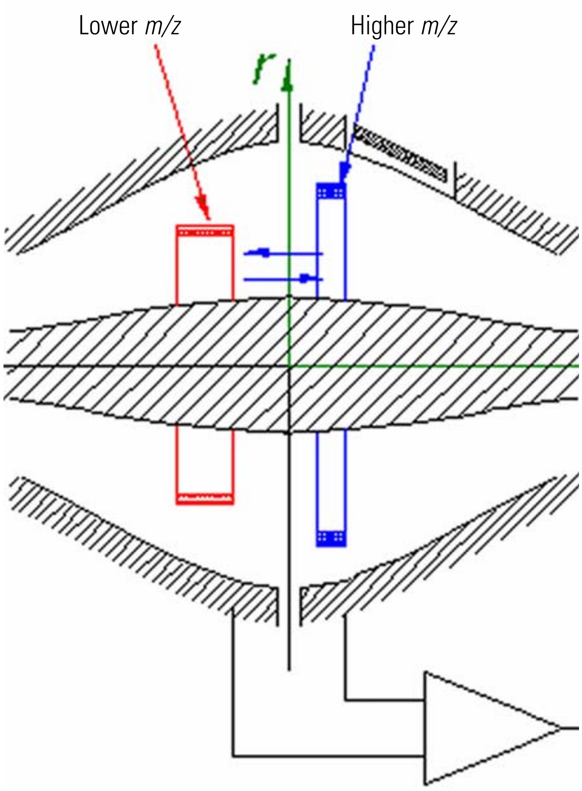


Figure 2-13. Approximate shape of ion packets of different *m/z* after stabilization of voltages

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 2-11 on page 2-14.) 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 2-13.) 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.

Active Temperature Control

Active temperature control is achieved by monitoring temperature directly on the Orbitrap analyzer assembly and compensating any changes in ambient temperature by a thermoelectric cooler (Peltier element) on the outside of the UHV chamber. A dedicated temperature controller board is used for this purpose. See page 2-60.

Peltier Cooling

To ensure stable operating conditions in the UHV chamber, it can be cooled or heated (outgassing) by means of a Peltier element on the outside. A second Peltier element is on the back of the CE power supply board. See Figure 2-41 on page 2-58.

The Peltier cooling is based on the Peltier Effect, which describes the effect by which the passage of an electric current through a junction of two dissimilar materials (thermoelectric materials) causes temperature differential (cooling effect). The voltage drives the heat to flow from one side of the Peltier element to the other side, resulting in cooling effects on one side and heating effects on the other side.

To remove the heat from the hot side of the Peltier elements, they are connected to the cooling water circuit of the Orbitrap Elite mass spectrometer. See "Cooling Water Circuit" on page 2-41 for further information.

HCD Cell

The HCD cell 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 collision gas to provide increased gas pressure inside the multipole. See “Gas Supply” on page 2-37 for details. The ETD Ion Optic Supply board provides the voltages for the HCD cell. (See page 2-46.)

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 fragment spectra generated in the HCD cell and detected in the Orbitrap analyzer show a fragmentation pattern comparable to the pattern of typical triple quadrupole spectra. See the *Orbitrap Elite Getting Started* manual for more information.

HCD and ETD

In the Orbitrap Elite ETD mass spectrometer, ETD reagent anions can efficiently pass through the high pressure region of the HCD cell. This is an important prerequisite to allow for a fast switching (that is, scan to scan) between HCD and ETD fragmentation, thus making comparative measurements possible. When compared with the standard Orbitrap Elite MS, HCD performance is not in any way compromised by the addition of the ETD Module.

ETD System

In the Orbitrap Elite ETD mass spectrometer, an ETD Module is physically coupled to the back of the Orbitrap Elite MS. See Figure 2-14. A quadrupole mass filter replaces the octapole of the Orbitrap Elite MS. See Figure 2-2 on page 2-3. The linear trap provides the voltages for the quadrupole mass filter. A tube, which contains the transfer multipole, connects the HCD housing to the ETD Module. See Figure 2-22 on page 2-30. The ETD Ion Optic Supply board is mounted on top of the data acquisition unit on the right side of the instrument. See Figure 2-33 on page 2-46.

Figure 2-14. Orbitrap Elite ETD MS front view

Protein or peptide analyte ions may also be fragmented in the linear trap by negatively charged reagent ions (fluoranthene radical anions) from the reagent ion source (ETD Module). These negatively charged ions transfer electrons to protein or peptide analyte ions and cause them to fragment at their peptide bonds to produce c and z type fragments (versus the y and b fragments produced by CID). The resulting analyte fragment ions provide another way of analyzing these molecules as compared to CID and PQD. Electron Transfer Dissociation (ETD) improves the identification of important post-translational modification (PTM) for characterization.

NOTICE Among others, the ETD system is also available as an upgrade on existing Velos Pro and Orbitrap Elite systems. ▲

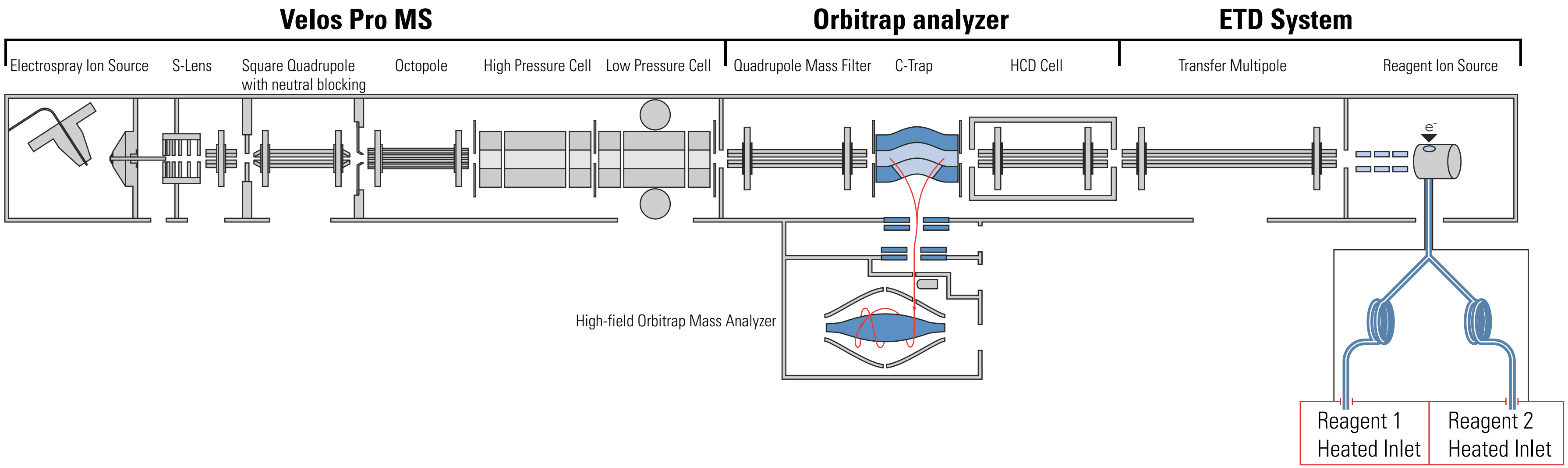


Figure 2-15. Schematic of the Orbitrap Elite ETD MS

Principle of Operation

During a typical ETD MS/MS scan, analyte cations are injected into the linear trap for subsequent precursor cation isolation. Then, ETD reagent anions are generated in the CI ion source and are transferred into the linear trap via RF-only ion guides (transfer multipoles), the gas-filled HCD cell, and the C-Trap. (See Figure 2-15 on page 2-20.)

The reagent ions pass a quadrupole mass filter between C-Trap and linear trap. This ion guide works as a low pass mass filter to remove the adduct ions of the fluoranthene radicals and molecular nitrogen at *m/z* 216. These adduct ions favor proton transfer reactions instead of electron transfer.

The application of a supplementary RF voltage on the end lenses of the linear trap allows ions of opposite polarity to be trapped in the same space at the same time (charge-sign independent trapping—CSIT).

During ion-ion reactions in the linear trap, electrons are transferred from the reagent anions to the precursor cations. The resulting product ions are mass-to-charge (*m/z*) analyzed in either the linear trap (if speed and sensitivity are important) or the Orbitrap analyzer (if mass resolution and mass accuracy are important).

ETD Module

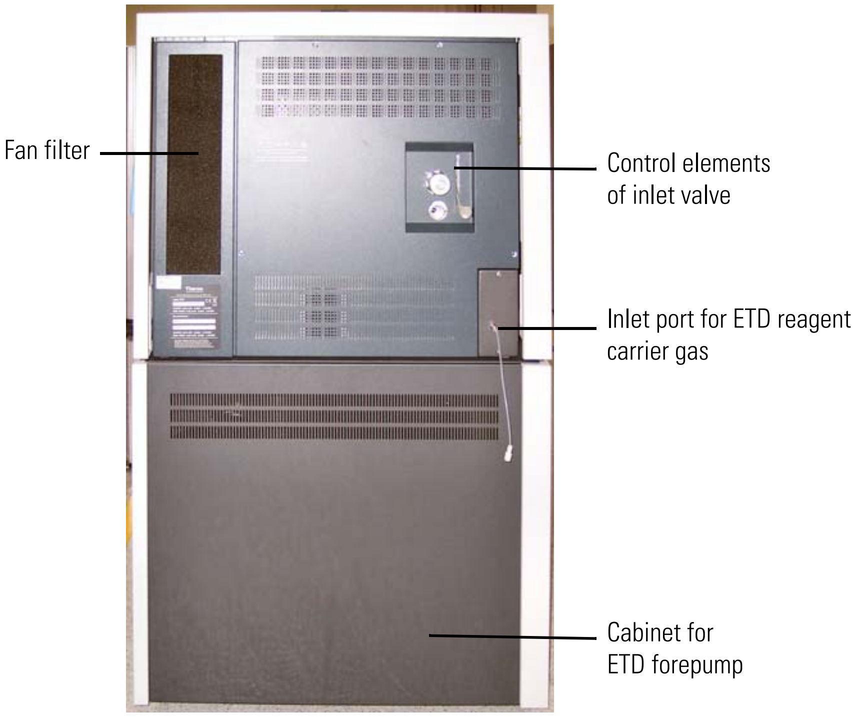
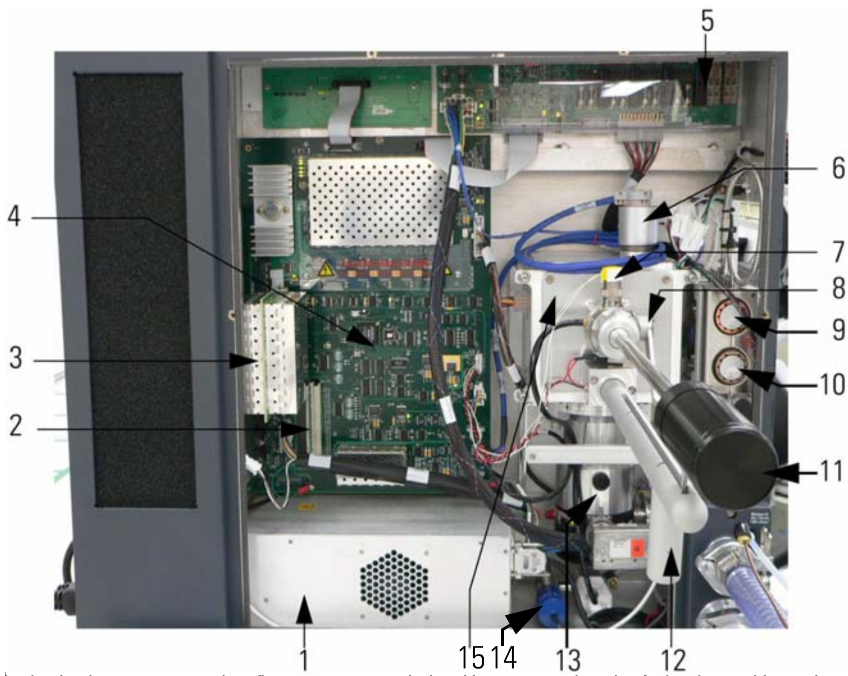


Figure 2-16. Orbitrap Elite ETD MS, rear side



Labeled components: 1=power module, 2=connector to Interface Board (Interface Board is behind the ETD Control PCB, item #4), 3=DC HV Supply PCB, 4=ETD Control PCB, 5=Heater Control PCB, 6=ion gauge, 7=inlet valve solenoid, 8=inlet valve lever in closed (down) position, 9=reagent heater 1, 10=reagent heater 2, 11=ion volume tool handle, 12=guide bar, 13=TMP, 14=Convectron™ gauge, 15=vacuum manifold (contains ion source and ion volume)

Table 2-3. Rear view of the ETD Module, with major component locations

Figure 2-16 shows the rear side of the ETD Module. It consists of the reagent ion source, ETD Module electronics, ETD Module power supply, ETD Module forepump, and the hardware that connects the ETD Module to the mass detectors.

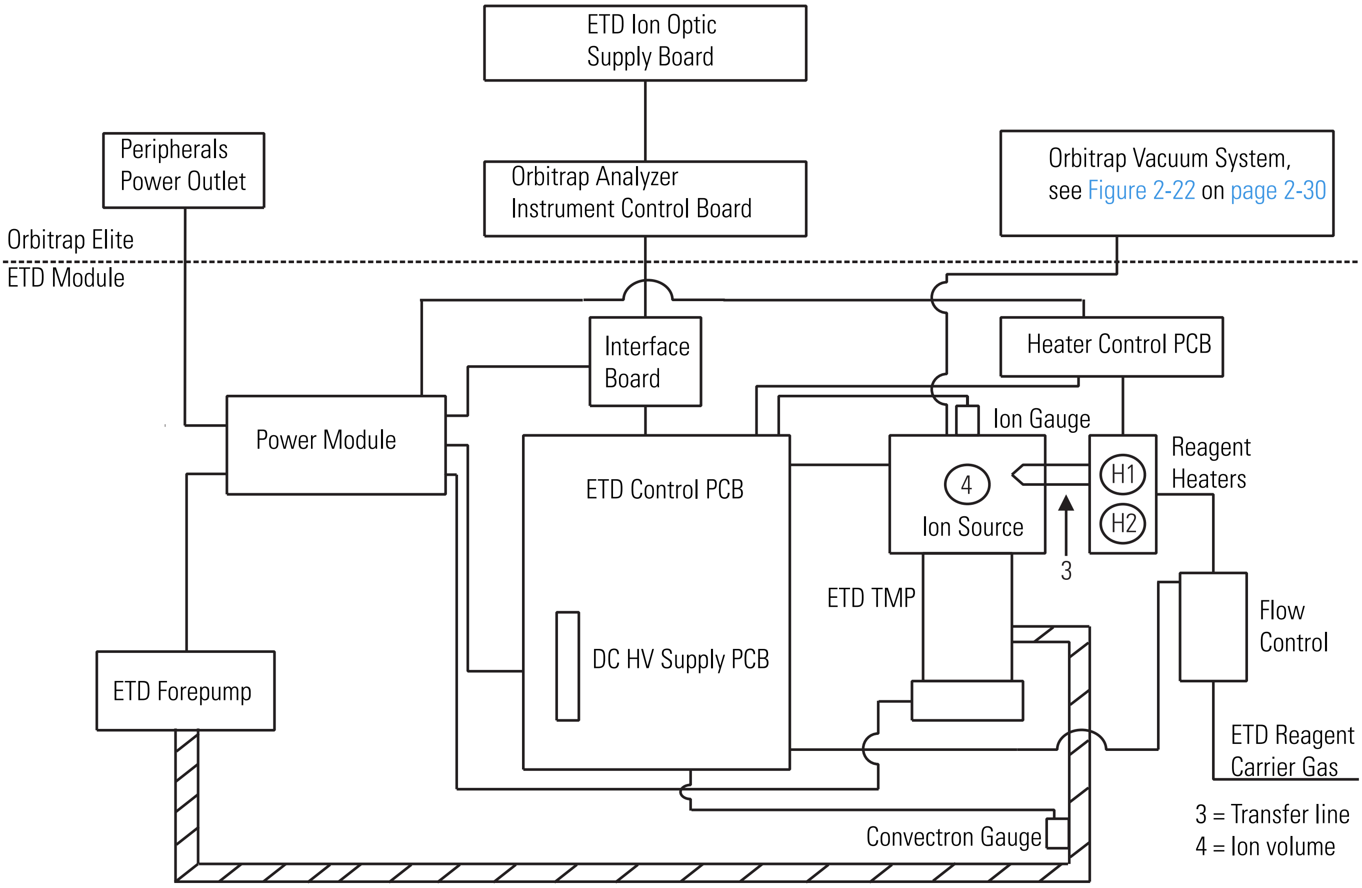


Figure 2-17. ETD Module functional block diagram

The following sections describe the major ETD Module components that are shown in Figure 2-3 on page 2-22 and Figure 2-17.

ETD Power Module

The ETD power module (item #1 in Figure 2-3) receives 220 V, 10 A, from the peripherals power outlet. See Figure 2-9 on page 2-10. It distributes appropriate voltages and currents to the ETD components. It also contains DC power supplies.

ETD Module Power Panel

The external receptacles and switches for the power module are on the ETD power module panel at the right side of the ETD Module. See Figure 2-18.

Figure 2-18. Right side of the Orbitrap Elite ETD MS

Figure 2-19 shows a close up picture of the ETD Power Module panel. Power In is connected to the peripherals power outlet of the MS portion. See Figure 2-9 on page 2-10. Forepump is a receptacle to power the ETD forepump (220 V AC, 5 A).

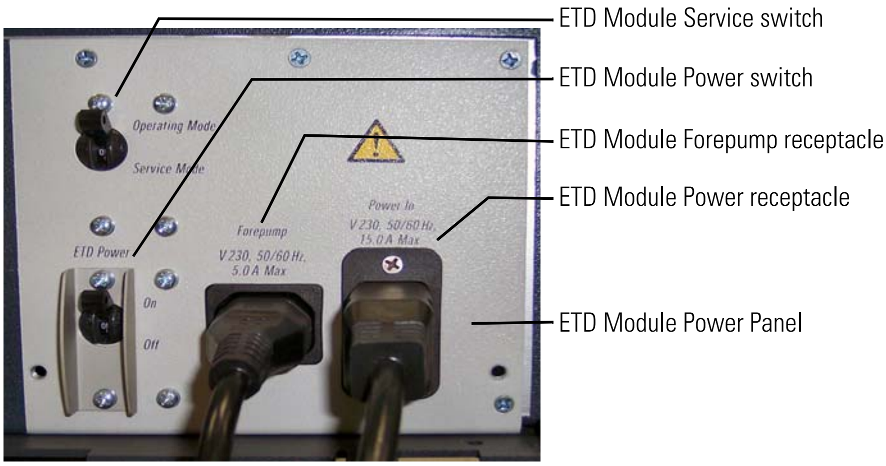


Figure 2-19. ETD Power Module panel

The ETD power module panel contains the main breaker and the service switch for the ETD Module. During normal operation, the ETD Power switch is left On and the service switch is left in the Operating Mode position. As a safety feature, both components of the Orbitrap Elite ETD system (the mass spectrometer and the ETD Module) are shut down with one set of switches, the mass spectrometer switches. When you perform maintenance on components inside the ETD Module as described in "Maintenance of the ETD Module" on page 6-15, you set the mass spectrometer's service switch to the Service position. The service switch turns On or Off power to all ETD Module components except turbomolecular pump and forepump.

ETD Module Interface Board

The ETD Module Interface board (item #2 in Figure 2-3 on page 2-22) provides an electronic interface between the ETD Module and the MS. This board also allows the power to both the MS and the ETD Module to be controlled by the MS power control panel switches:

- The MS Main Power switch controls the power supply to all components in both the MS and the ETD Module.
- The MS FT Electronics switch controls the power supply to all mass spectrometer and ETD Module components except the pumps that are connected to the MS and the ETD Module.

NOTICE The ability to control the power to both components of the Orbitrap Elite ETD mass spectrometer at one point (the power control panel switches of the MS) is a safety feature. ▲

ETD Control PCB

The ETD Control PCB (item #4 in Figure 2-3) controls most of the ETD Module functions. The ETD Control PCB consists of circuits that control:

- ETD Module operating logic
- Ion source (filament, ion source heater, lenses)
- Heater temperature and readback logic (for reagent heaters, transfer line heater, and the restrictor oven heater)
- Reagent gas flow
- Oven cooling gas control
- Ion gauge
- Convectron™ gauge

The DC HV Supply PCB (item #3 in Figure 2-3 on page 2-22) is plugged in to the ETD Control PCB.

ETD Heater Control PCB

The ETD Module Heater Control PCB (item #6 in Figure 2-3) contains the power source and temperature sensing circuitry for the four heaters in the reagent ion source. The heaters are H1 and H2 (the two reagent heaters, Figure 2-17 on page 2-23, and items #9 and #10 in Figure 2-3), the transfer line heater (#3 in Figure 2-3), and the restrictor oven heater (not shown in Figure 2-3). The Heater Control PCB reports temperature information to the heater temperature and readback logic on the ETD Control PCB. The heater temperature and readback logic controls how the Heater Control PCB applies power to the ETD Module heaters.

Reagent Carrier Gas Flow Control for ETD

The ETD Module contains a digital flow control for the chemical ionization (CI) gas/reagent carrier gas provided by the ETD Control PCB (See Figure 2-3 on page 2-22.) and an electronic pressure regulator. The gas serves two functions in the ETD Module:

- As a carrier gas, the nitrogen sweeps the reagent (fluoranthene) from the vial to the ion source where the reagent radical anions are formed.
- As a chemical ionization (CI) vehicle, the nitrogen undergoes collisions with 70 eV electrons from the filament in the ion volume. These 70 eV electrons from the filament knock electrons off of the nitrogen molecules (nitrogen ions are created). The secondary electrons resulting from these collisions have near thermal kinetic energies. These thermal electrons are captured by the fluoranthene to form reagent radical anions that react with the analyte.

Thermo Fisher Scientific strongly recommends a mixture of 25% helium and 75% nitrogen. The helium in this mixture serves as a tracer gas to enable leak checking of gas connections using conventional thermal conductivity-based leak detectors, which are widely used to check leaks in gas chromatography equipment. See "Gas Supply of the Reagent Ion Source" on page 2-39 for detailed information.

The reagent carrier gas supply in the laboratory is connected to the ETD reagent carrier gas port at the rear side of the ETD Module. See Figure 2-29 on page 2-39.

Reagent Heaters

The reagent heaters (items #9 and #10 in Figure 2-3 on page 2-22, H1 and H2 in Figure 2-17 on page 2-23) heat the reagent to obtain a sufficient amount of reagent vapor in the carrier gas. The reagent heaters are powered by the Heater Control PCB which, in turn, is controlled by the ETD Control PCB.

The reagent heaters are turned on by selecting the Reagent Ion Source On check box in the Reagent Ion Source dialog box. See Figure 2-20.

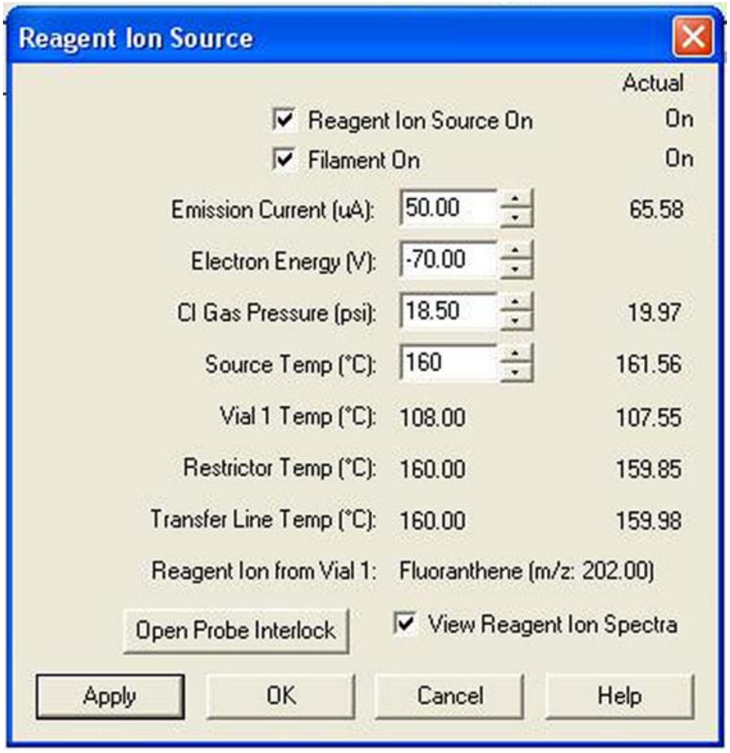


Figure 2-20. Reagent Ion Source dialog box

When you deselect the Reagent Ion Source On check box, the reagent heaters and filament immediately turn off and the reagent ion source goes into Standby mode.

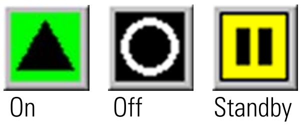
When the reagent ion source is placed in Off mode, cooling nitrogen (high-purity nitrogen) will turn on. This is confirmed by an audible rush (hissing noise) of nitrogen from the reagent ion source area in the back of the ETD Module. This is normal operation. See also “Turning off the Reagent Ion Source: What to Expect” on page 5-14.

The nitrogen cooling gas turns off when the reagent heaters reach 70 °C. If it is necessary to install or replace the reagent vials, then follow the procedure in “Replacing the Reagent Vials” on page 6-50.

NOTICE The rushing or hissing noise of the nitrogen that comes from the back of the ETD Module will stop when the cooling nitrogen turns off. ▲

When the reagent heaters are in Standby mode, they are immediately turned on by selecting the Reagent Ion Source On check box (Figure 2-20 on page 2-27). When starting from room temperature, it takes up to ten minutes for the reagent heaters and vials to stabilize at 108 °C and reagent to be delivered to the ion source.

NOTICE When you switch on a cold reagent ion source, the Tune Plus software warns you that the vial temperature is not sufficient. The filament is automatically switched on after the temperature has stabilized. ▲



When you click the **Standby** button in the Tune Plus window (shown in the left margin), you initiate a Standby process. It delays turning off the reagent heaters and the start of nitrogen cooling for one hour after the system is placed in Standby. This method of placing the system in Standby permits a quick return to operation after a break (lasting one hour or less) rather than waiting up to ten minutes for the heaters to return to temperature and reagent delivery to be fully restored.

In summary:

- The reagent heaters turn off immediately when the Reagent Ion Source On check box is deselected in the Reagent Ion Source dialog box. (See Figure 2-20 on page 2-27.)
- The reagent heaters turn off one hour after the system is placed in Standby by clicking the Standby button in the Tune Plus window.

Reagent Ion Source

The ion source (Figure 2-3 on page 2-22 and inside of the vacuum manifold, see item #14 in Figure 2-3) is where the reagent ions are formed. The ion source contains the filament, the reagent ion volume, and the ion source heater. The filament is the source of electrons that react with the reagent to form reagent ions. The reagent ion volume is the space where this reaction takes place. See Figure 2-21. The ion source heater is controlled by the ETD Control PCB.

The reagent ion source contains two reagent vials, CI/carrier gas (nitrogen) handling hardware and flow restrictors, ion volume and filament, ion optics, and heaters for these components. The flow restrictors keep the internal pressure of the reagent vials below atmospheric pressure. This prevents the contents of the reagent vials from being expelled to the laboratory atmosphere.

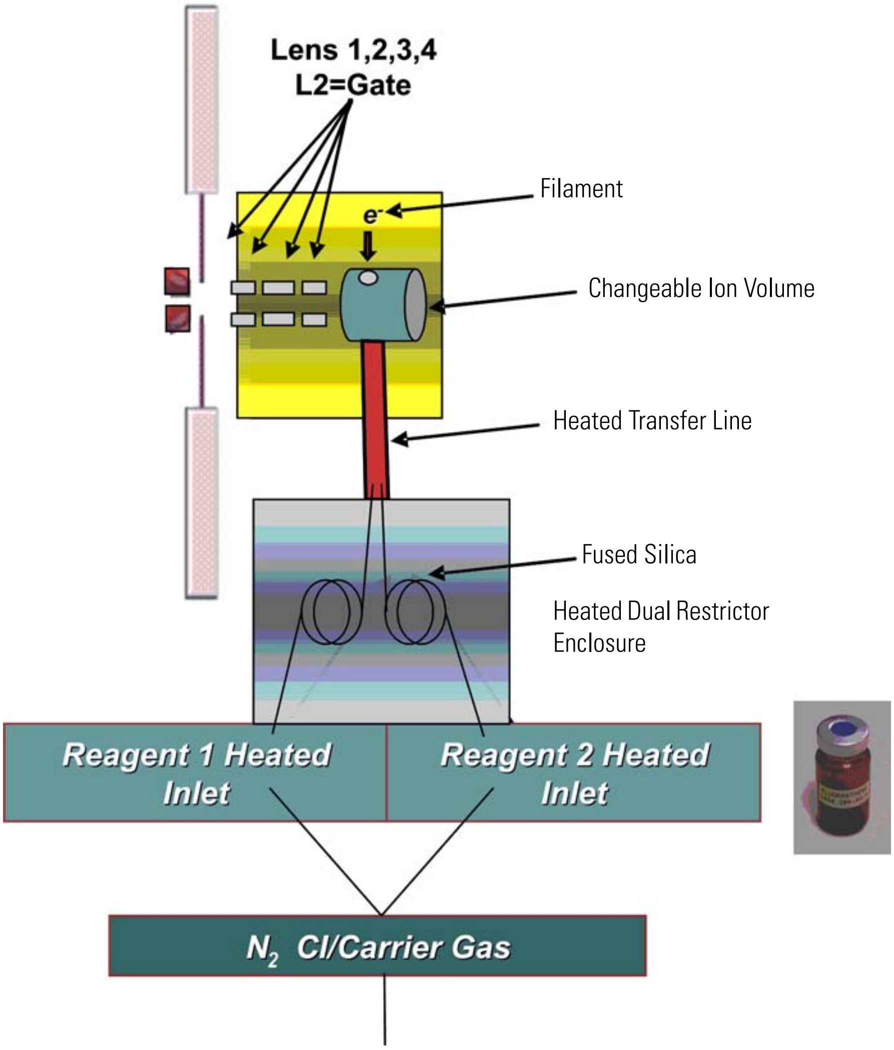


Figure 2-21. Reagent ion source schematics

Vacuum System

Figure 2-22 shows a schematical overview of the Orbitrap analyzer vacuum system.

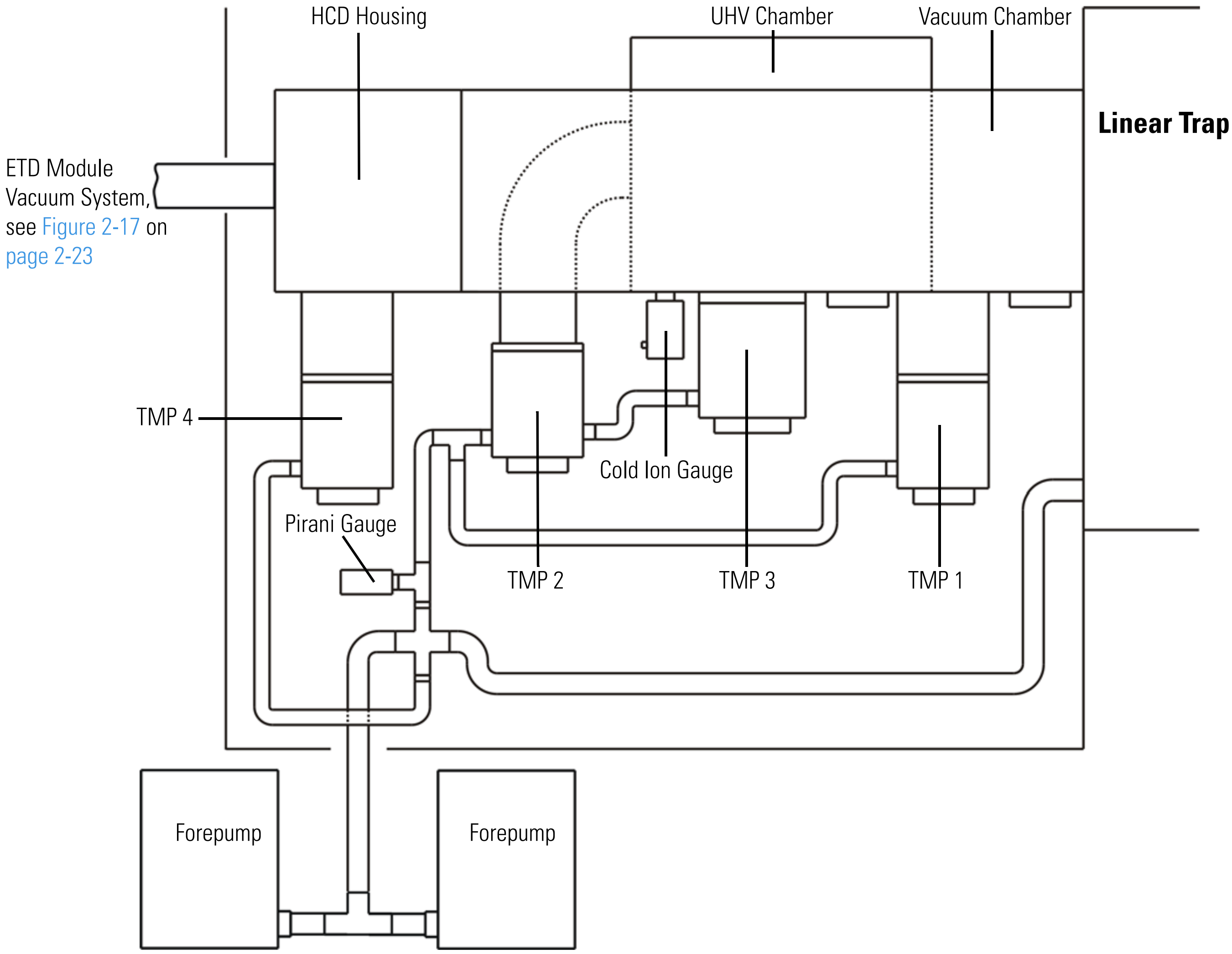


Figure 2-22. Schematic of Orbitrap analyzer vacuum system (CLT compartment and Orbitrap chamber not shown)[a]

[a] For an abridged version of the parts list, see page 7-3.

The Orbitrap Elite mass spectrometer has the following vacuum compartments:

- **CLT compartment in the aluminum vacuum chamber** (pumped by the same pump as the linear trap)
- **Vacuum chamber** (pumped by a water-cooled 60 L/s—for N_2—turbomolecular pump HiPace™ 80, *TMP 1*, manufacturer: Pfeiffer)
- **Ultra high vacuum chamber** (UHV chamber, pumped by a water-cooled 60 L/s turbomolecular pump HiPace 80, *TMP 2*, manufacturer: Pfeiffer)

- **Orbitrap chamber** (pumped by a 260 L/s—for N_2—water-cooled turbomolecular pump HiPace 300, *TMP 3*, manufacturer: Pfeiffer)
- **HCD housing** (pumped by a water-cooled 60 L/s turbomolecular pump HiPace 80, *TMP 4*, manufacturer: Pfeiffer)

The forepumps of the linear trap provide the forevacuum for the turbomolecular pumps TMP 1 to TMP 4.

Turbomolecular Pumps

All parts of the system except for the Orbitrap analyzer are mounted in a aluminum vacuum chamber that is evacuated by a 60 L/s turbomolecular pump (TMP 1, see Figure 2-23). The rotary vane pumps of the linear trap (see page 2-33) provide the forevacuum for this pump. This chamber is bolted to a stainless steel welded UHV chamber, which accommodates Orbitrap analyzer, lenses, and corresponding electrical connections.

Figure 2-23. Vacuum components on the left instrument side

The UHV chamber is evacuated down to 10^{-8} mbar pressure range by a 60 L/s UHV turbomolecular pump (*TMP 2*, see Figure 2-24 on page 2-32). The Orbitrap analyzer itself is separated from the UHV chamber by differential apertures and is evacuated down to 10^{-10} mbar by a 260 L/s turbomolecular pump (*TMP 3*, see Figure 2-24). The HCD housing is evacuated by a 60 L/s UHV turbomolecular pump *(TMP 4*, see Figure 2-23) that is mounted to its bottom via an elbow. This dedicated pump for the HCD cell protects the low pressure cell of the linear trap from gas overload.

In the Orbitrap Elite ETD mass spectrometer, a tube that contains the transfer multipole (flatapole) connects the HCD housing to the ETD Module.

Figure 2-24. Vacuum components on the right instrument side

All turbomolecular pumps have TC 110 control units (manufacturer: Pfeiffer). A 24 V switch mode power supply provides the electric power for all four turbomolecular pumps of the system.

Linear Trap Turbomolecular Pump

A separate turbomolecular pump provides the high vacuum for the linear ion trap. It it is mounted to the bottom of the vacuum manifold of the linear ion trap. For more information, refer to the *LTQ Series Hardware Manual*.

ETD Module Turbomolecular Pump

In the Orbitrap Elite ETD mass spectrometer, a dedicated turbomolecular pump (Edwards EXT75DX) provides the high vacuum for the ETD reagent ion source. See Figure 2-3 on page 2-22. It is backed up by a dedicated rotary vane pump at the bottom of the ETD Module. See Figure 2-26 on page 2-34. This air-cooled turbomolecular pump contains no user-serviceable parts.

Forepumps of the Linear Trap

The rotary vane pumps from the linear trap serve as forepumps for the three smaller turbomolecular pumps (TMP 1, TMP 2, and TMP 4). The exhaust hose from the forepumps is led to the back of the instrument and connects them to the exhaust system in the laboratory. The forepumps stand on a small cart in the forepumps cabinet below the linear trap. See Figure 2-25.

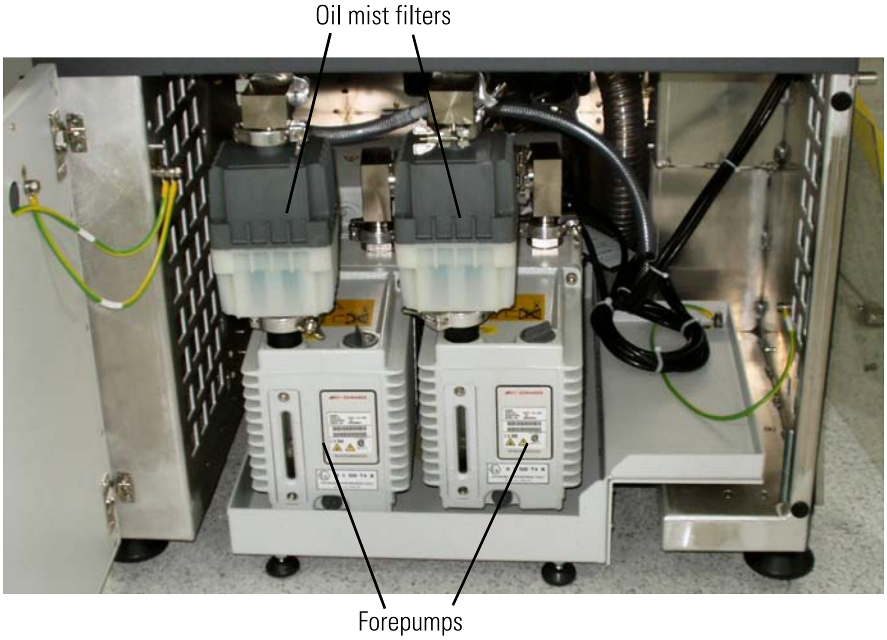


Figure 2-25. Forepumps cabinet

To minimize the ingress of pump oil into the exhaust system, the outlets of the forepumps are fitted to oil mist filters. See page 6-14 on instructions about returning the collected oil to the forepumps.

The forepumps of the linear trap are powered by the power panel of the linear ion trap.

Leave the switches of the forepumps always in the On position to provide the control from the vacuum control panel. Before starting the pumps, however, make sure that:

- The forevacuum pumps are filled with oil,
- They are connected to the power supply, and
- The gas ballast is shut.

For a detailed description of the forepumps, refer to the handbook of the manufacturer.

Forepump of the ETD Module

In the Orbitrap Elite ETD mass spectrometer, a rotary vane pump (Edwards RV 3) provides the forevacuum for the ETD turbomolecular pump. (See “ETD Module Turbomolecular Pump” on page 2-32.) It stands in a cabinet at the bottom of the ETD Module. The ETD forepump has an oil mist filter and stands on a drip pan. See Figure 2-26.

An exhaust hose connects the forepump to the exhaust system in the laboratory. A forevacuum tube connects the ETD forepump to the ETD TMP. The forepump electrical cord is plugged into the Forepump receptacle on the ETD Module power panel. See Figure 2-19 on page 2-24.

For maintenance instructions for the ETD forepump, see “Maintenance of the ETD Forepump” on page 6-7 and the manual that came with the forepump.

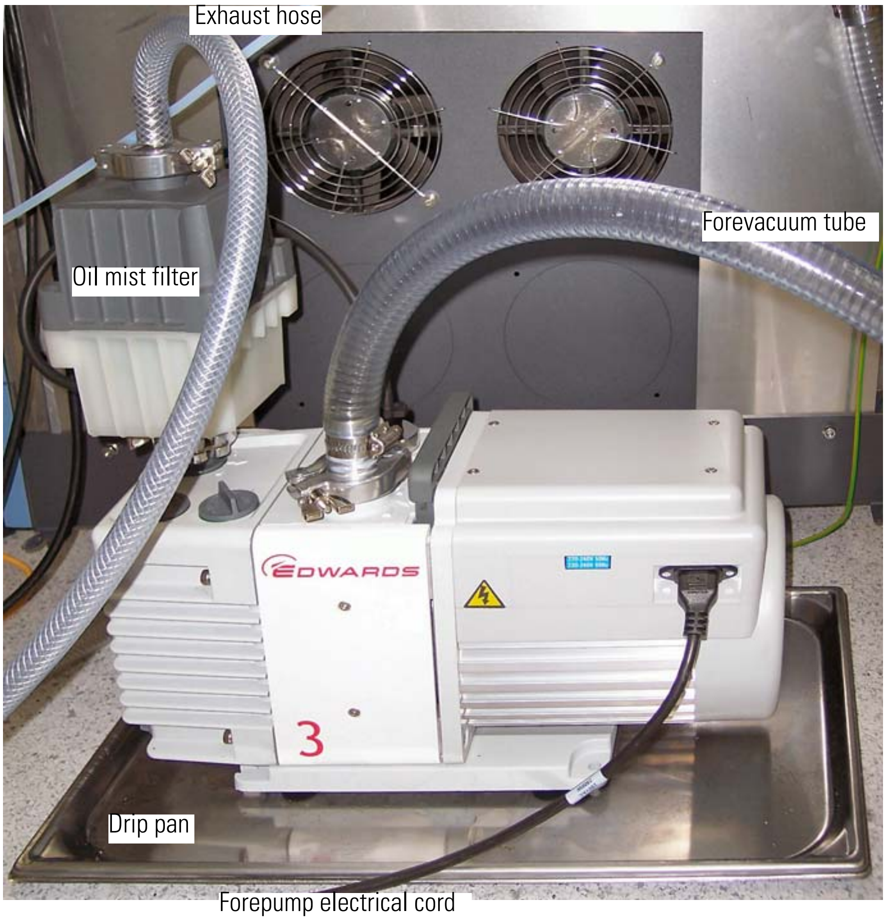


Figure 2-26. Forepump for ETD Module

Vacuum System Controls

The power distribution board controls all turbomolecular pumps by voltage levels. See “Power Distribution Board” on page 2-52. An interface for RS485 data by the instrument control board connects the turbomolecular pumps with the linear ion trap. (See “Instrument Control Board” on page 2-51.) The turbomolecular pump of the linear ion trap and the ETD turbomolecular pump have individual controllers.

Vacuum Gauges

Several vacuum gauges monitor the vacuum within the instrument:

- The forevacuum of the Orbitrap Elite mass spectrometer is monitored by an Active Pirani gauge (TPR 280, manufacturer: Pfeiffer) connected to the forevacuum line. See Figure 2-23 on page 2-31.
- The high vacuum of the Orbitrap Elite mass spectrometer is monitored by a Cold Ion Gauge (IKR 270, manufacturer: Pfeiffer) connected to the UHV chamber. See Figure 2-24 on page 2-32. Because the gauge would be contaminated at higher pressures, it is switched on only when the forevacuum has fallen below a safety threshold ($<10^{-2}$ mbar).
- The linear ion trap vacuum is monitored by a Convectron™ gauge and an ion gauge. Refer to the *LTQ Series Hardware Manual* for more information.
- In the Orbitrap Elite ETD mass spectrometer, two dedicated vacuum gauges monitor the vacuum in the ETD Module. A Convectron gauge (see Figure 2-3 on page 2-22 and Figure 2-17 on page 2-23) monitors the pressure in the ETD forevacuum line and an ion gauge (see Figure 2-3) monitors the pressure in the reagent ion source. Table 2-4 shows typical pressure readings in the ETD Module.

Table 2-4. Typical pressure readings in the ETD Module

Conditions	Convection Gauge Reading	Ion Gauge Reading
CI gas pressure set to 20 psi	0.1–0.01 Torr	$20–35\times10^{-5}$ Torr

The vacuum gauges of the Orbitrap Elite mass spectrometer are connected to the power distribution board that directly responds to the pressure values. (See “Power Distribution Board” on page 2-52.) The analog values are digitized by the instrument control board. (See “Instrument Control Board” on page 2-51.) They are then sent as readout values to the data system.

Switching on the Vacuum System

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

1. After the Vacuum Pumps switch is switched On, the pumps of the linear ion trap and the Orbitrap Elite mass spectrometer are run up. The Pirani gauge (see above) controls the Orbitrap Elite MS low vacuum pressure as well as the pressure at the forevacuum pumps. Within a short time, a significant pressure decrease must be observed. The goodness of the vacuum can be estimated by means of the rotation speed of the turbomolecular pumps (for example, 80% after 15 minutes).

2. If the working pressure is not reached after the preset time, the complete system is switched off. At the status LED panel of the power distribution board, an error message (Vacuum Failure) is put out (see below).

3. The Cold Ion Gauge is only switched on after the low vacuum is reached. It is then used to monitor the vacuum in the Orbitrap analyzer region.

Vacuum Failure

In case the pressure in the Orbitrap Elite mass spectrometer or the linear ion trap exceeds a safety threshold, the complete system including linear ion trap, electronics, and pumps is switched off. However, the power distribution is kept under current and puts out an error message at the LED panel. (See “Power Distribution Board” on page 2-52.) It can be reset by switching the main power switch off and on. (See “Main Power Switch” on page 2-9.)

Upon venting, the vent valves of the turbomolecular pumps on the Orbitrap analyzer stay closed. Only the vent valve of the linear ion trap is used. (See “Vent Valve of the Linear Ion Trap” on page 2-39.)

Vacuum System Heating during a System Bakeout

After the system has been open to the atmosphere (for example, for maintenance work), the vacuum deteriorates due to contaminations of the inner parts of the vacuum system caused by moisture or a power outage. These contaminations must be removed by heating the vacuum system: a system bakeout. See “Baking Out the System” on page 6-6.

Gas Supply

This section describes the gas supplies for the mass analyzers of the Orbitrap Elite mass spectrometer and the reagent ion source of the Orbitrap Elite ETD MS.

Gas Supply for the Mass Analyzers

Figure 2-27 shows a schematical view of the gas supply for the instrument. The gas supply of the ETD system is highlighted in gray.

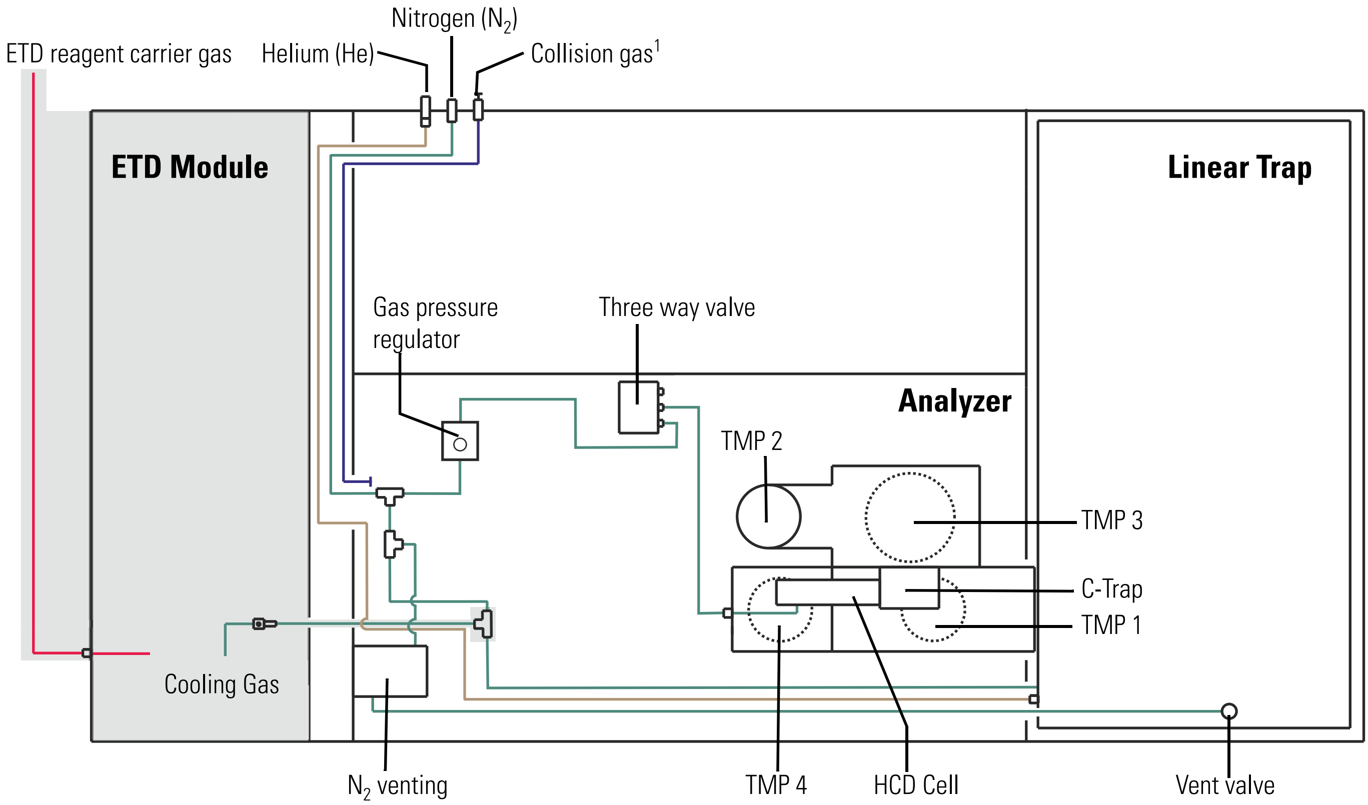


Figure 2-27. Schematic of gas supply for Orbitrap Elite ETD MS[a]

[a] For parts lists of the gas supply, see page 7-4 and page 7-5.

Gas Inlet Ports of the Instrument

On its right side (See Figure 2-9 on page 2-10.), the instrument provides three gas inlet ports for the gas supply of the mass analyzers:

- Nitrogen: The linear trap requires high-purity (99%) nitrogen for the API sheath gas and auxiliary/sweep gas. The required gas pressure is 690 ± 140 kPa (6.9 ± 1.4 bar, 100 ± 20 psi).

[1] The port named Collision Gas is not used in the Orbitrap Elite MS.

In the Orbitrap Elite ETD mass spectrometer, the ETD system uses the high-purity nitrogen for cooling the reagent vials when the reagent ion source is turned off.

- Helium: The linear trap requires ultra-high purity (99.999%) helium for the collision gas. The required gas pressure is 275 ± 70 kPa (2.75 ± 0.7 bar, 40 ±10 psi).

Gas Distribution Within the Instrument

Helium gas is led from the helium port through a stainless steel capillary to the right rear side of the linear trap. See Figure 2-27 on page 2-37. High purity nitrogen gas is led from the nitrogen port via Teflon tubing to the right side of the Orbitrap Elite mass spectrometer. Here, two T-pieces divide the nitrogen gas flow into three parts.

The first part of the high purity nitrogen gas flow is directed through Teflon tubing via a pressure regulator to the vent valve of the linear trap. (See Figure 2-28.) The second part of the nitrogen flow is directed through Teflon tubing to the API source. The third part of the nitrogen flow enters a gas pressure regulator, by which the instrument controls the gas pressure to the C-Trap and HCD collision cell. (See Figure 2-28, background.) From the regulator, the collision gas is led through PEEKSil™ tubing (75 µm ID silica capillary in 1/16 inch PEEK tubing) to the IN port of a three way valve. The gas leaves the valve through the OUT port and is led to the collision quadrupole next to the C-trap (flow rate: ~0.5 mL/min). The third port of the three way valve is closed. The valve is switched by the software through the power distribution board. The nitrogen gas that leaks from the HCD collision cell (3–5 mTorr) is used for ion trapping and cooling in the C-Trap.

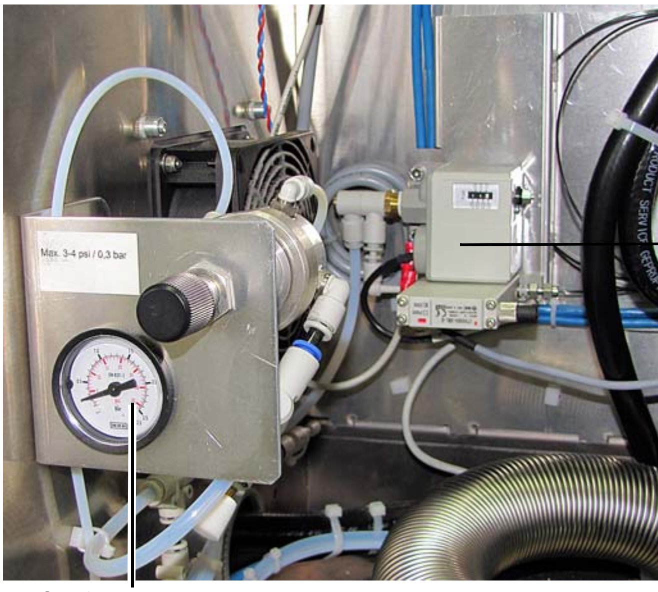


Figure 2-28. Gas regulators

In the Orbitrap Elite ETD mass spectrometer, nitrogen is also directed through Teflon tubing to the ETD Module to be used for cooling the reagent vials when the reagent ion source is switched off.

Vent Valve of the Linear Ion Trap

If the system and pumps are switched off, the system is vented. The vent valve is controlled by the linear ion trap. The *LTQ Series Hardware Manual* contains further information about the vent valve.

The instrument is vented with high purity nitrogen from the same tubing that supplies the Velos Pro MS sheath gas. See Figure 2-27 on page 2-37. The vent valve of the Velos Pro mass spectrometer is supplied by a pressure regulator that is set to a venting pressure of 3–4 psi. The pressure regulator is at the left side of the Orbitrap Elite mass spectrometer. (See Figure 2-28, front.)

Gas Supply of the Reagent Ion Source

In addition to high purity nitrogen for cooling, the reagent ion source of the Orbitrap Elite ETD mass spectrometer uses a mixture of 25% helium and 75% nitrogen gas as carrier gas and chemical ionization (CI) vehicle. This gas mixture must be ultra high-purity (minimum purity 99.999%) with less than 3.0 ppm each of water, oxygen, and total hydrocarbons. The required gas pressure is 690 ± 140 kPa (6.9 ± 1.4 bar, 100 ± 20 psi). The ETD carrier gas supply of the laboratory is connected by metal tubing to the inlet port at the rear side of the instrument. See Figure 2-29.

Figure 2-29. ETD reagent carrier gas port at the ETD Module

The helium in this mixture serves as a tracer gas to enable leak checking of gas connections with conventional thermal conductivity-based leak detectors, which are widely used to check leaks in gas chromatography equipment.

NOTICE If the helium/nitrogen mixture is not available, then use a nitrogen supply that is ultra high-purity (99.999%) with less than 3.0 ppm each of water, oxygen, and total hydrocarbons. ▲

Triple Gas Filter

A triple (oxygen/water/hydrogen) gas filter is installed between the regulator on the reagent carrier gas source and the ETD module to ensure that the reagent carrier gas (either nitrogen or helium/nitrogen) is better than 99.999% pure with much less than 1 ppm of oxygen, water, and hydrocarbons.

Refer to the filter manufacturer's instructions for information about how to monitor the color changes in the filters that indicate when the filters need to be replaced, as well as information about where to order new filters. If there are no leaks in the reagent carrier gas plumbing, then you can expect the filters to last a year or more. Thermo Fisher Scientific strongly recommends that a Thermo Fisher Scientific field service engineer replace the gas filters.

Cooling Water Circuit

A recirculating chiller (Thermo Scientific ThermoFlex™ 900) is shipped with the instrument and makes the mass spectrometer independent from any cooling water supply.

Figure 2-30 shows a schematical view of the cooling water circuit in the Orbitrap Elite mass spectrometer. Cooling water at a temperature of 20 °C enters and leaves the instrument at the bottom of the right side. See Figure 2-9 on page 2-10. First, the fresh water passes through the turbomolecular pumps in the order TMP 3 → TMP 1 → TMP 4 → TMP 2. Then it passes through the heating element (Peltier element) that maintains (±0.5 °C) the preset temperature of the analyzer. After that, the cooling water passes through the preamplifier cooling unit. Before it leaves the instrument, the water passes through the other Peltier element at the back of the central electrode power supply board.

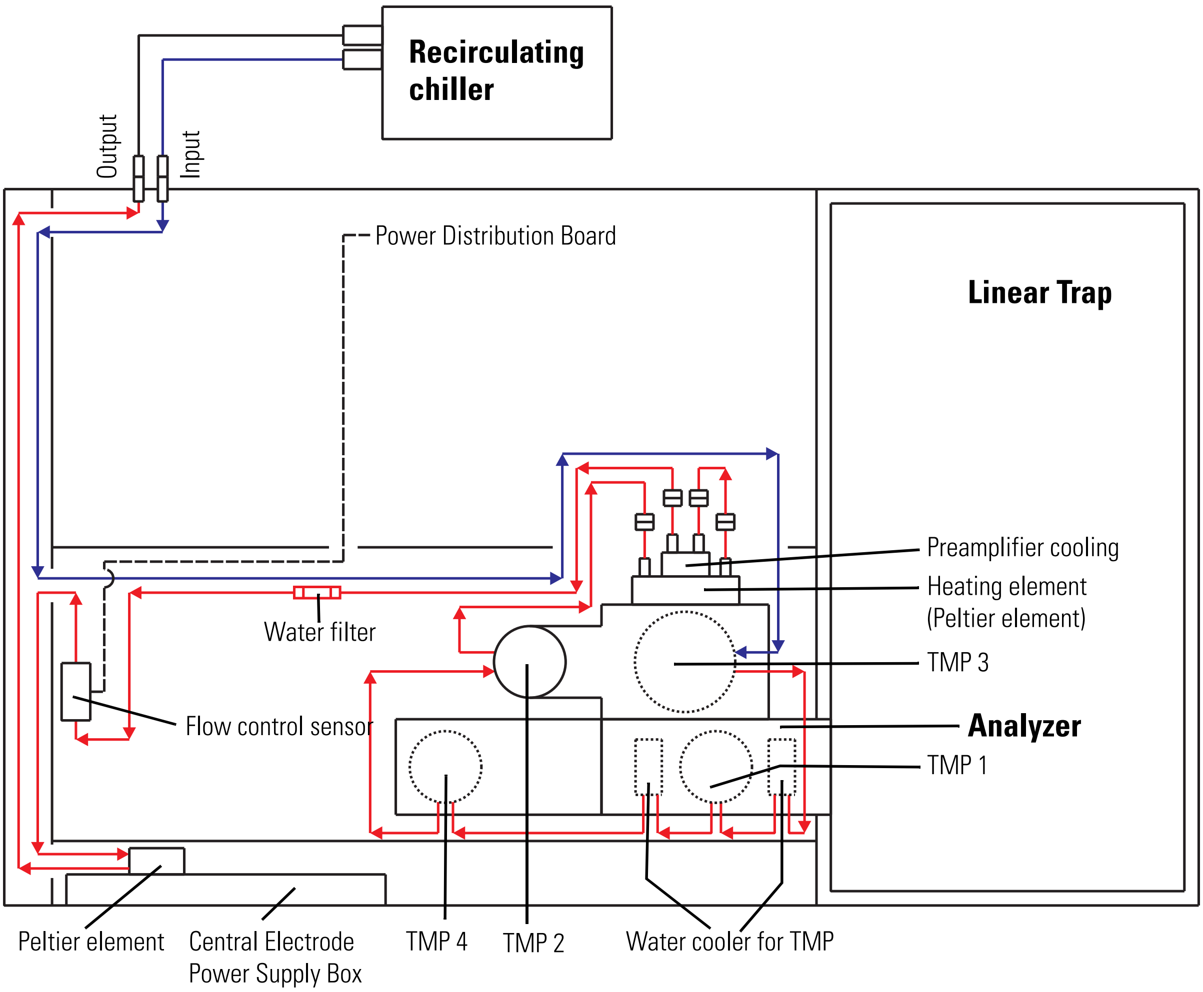


Figure 2-30. Schematic of cooling water circuit

A flow control sensor is connected to the power distribution board and allows displaying the current flow rate of the cooling water in the software. An inline filter, which is installed upstream, protects the sensor. It must be replaced annually, see page 6-60 for instructions.

For a parts list of the cooling water circuit, see page 7-4. For instruction about performing maintenance for the chiller, see "Maintenance of the Cooling Circuit" on page 6-60. See also the manufacturer's manual for the chiller.

Printed Circuit Boards

The Orbitrap Elite mass spectrometer is controlled by a PC running the Xcalibur™ software suite. The software controls all aspects of the instrument. The main software elements are the communication with the linear ion trap, the control of ion detection, and the control of the Orbitrap analyzer.

The following pages contain a short overview of the electronic boards in the MS portion of the Orbitrap Elite mass spectrometer. For each board, its respective location and function are given. If applicable, the diagnostic LEDs on the board are described. For a description of the printed circuit boards in the ETD Module, see "ETD Module" on page 2-22.

The electronics of the Orbitrap Elite 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. When replacing fuses, only use the correct type. Before calling a service engineer, please try to localize the defect via errors indicated in the software or diagnostics. A precise description of the defect will ease the repair and reduce the costs.

NOTICE Many of the electronic components can be tested by the Orbitrap Elite MS diagnostics, which is accessible from the Tune Plus window. ▲

Linear Ion Trap Electronics

The linear ion trap is connected to the Orbitrap Elite MS main power switch. The linear ion trap has a sheet metal back cover. Figure 2-31 shows the electronic connections at the rear side of the linear trap.

Figure 2-31. Electronic connections to linear trap

The linear ion trap electronics has two connections with the Orbitrap Elite MS electronics:

- Data communication with the internal computer of the Orbitrap Elite mass spectrometer. See "Electronic Boards on the Right Side of the Instrument" on page 2-45.

- Signal communication (SPI bus) with supply information for the instrument control board. See "Instrument Control Board" on page 2-51.

For further information about the linear ion trap electronics, refer to the *LTQ Series Hardware Manual.*

Electronic Boards on the Right Side of the Instrument

Figure 2-32 shows the parts of the instrument when the right side panel is opened. A transparent cover protects the lower part.

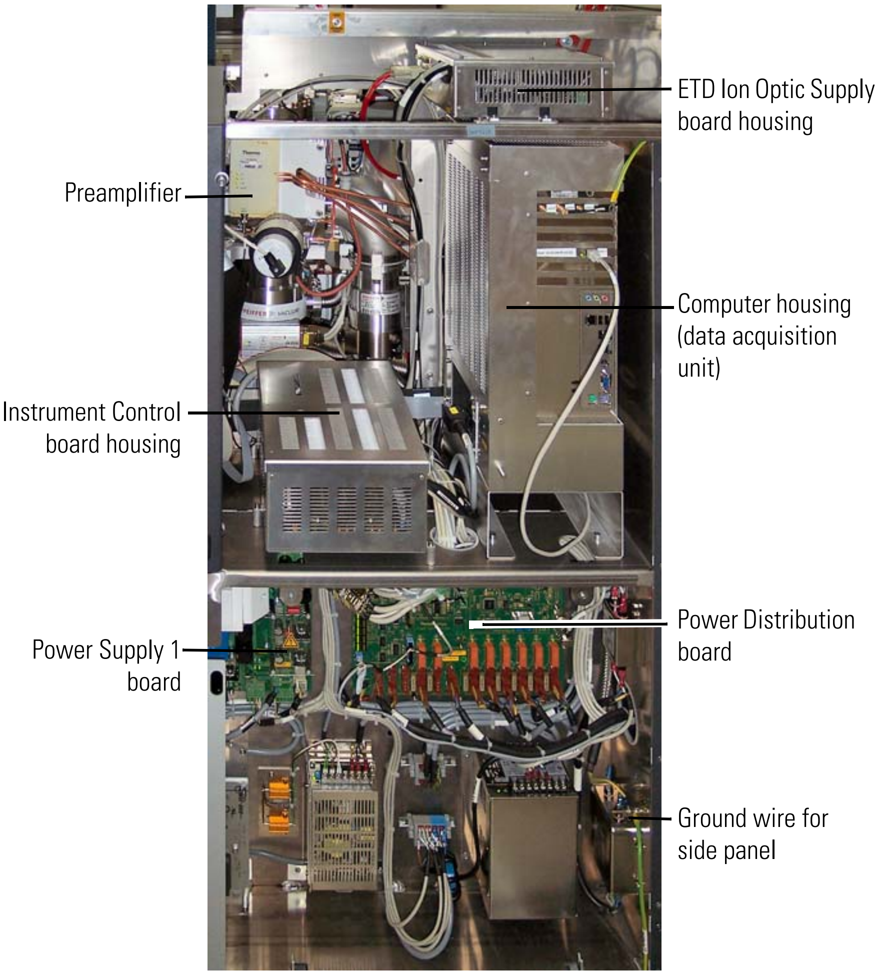


Figure 2-32. Electronic boards on the right side of the Orbitrap Elite MS

The side panel is connected to the instrument frame by two green/yellow ground wires. See bottom of Figure 2-32. The connectors on the panel are labeled with green-yellow PE (for **P**rotective **E**arth) signs. See photo left. Do not forget to reconnect them before closing the panel!

ETD Ion Optic Supply Board

The ETD Ion Optic Supply board is mounted on top of the data acquisition unit. See Figure 2-33. It supplies the voltages for the HCD cell. In the Orbitrap Elite ETD mass spectrometer, this board also supplies the RF voltage and the DC voltages for the ETD Module: an RF voltage with DC offset, three DC voltages with ±250 V, and a DC voltage with ±12 V.

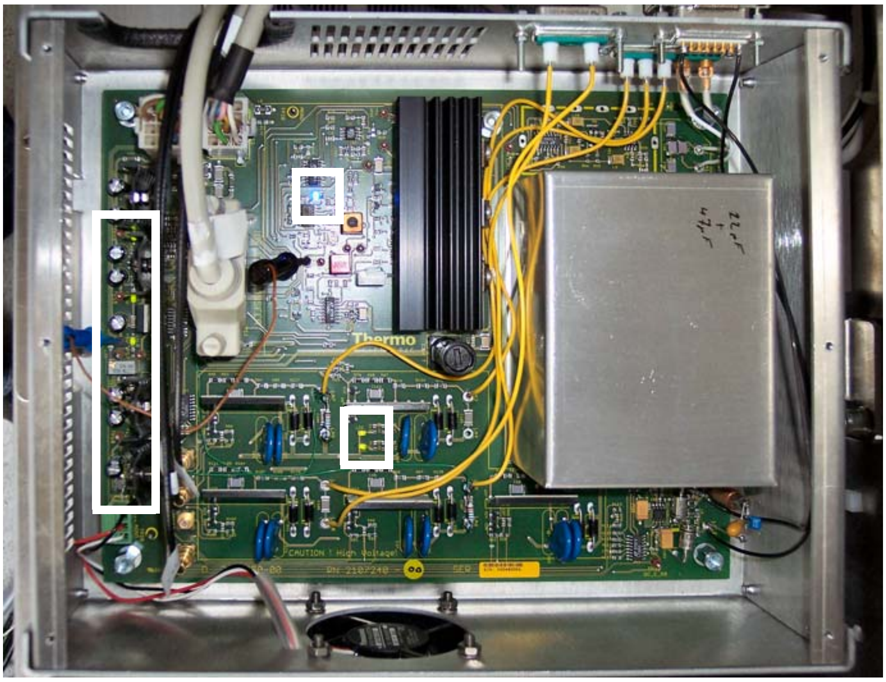


Figure 2-33. ETD Ion Optic Supply board

The diagnostic LEDs on the ETD ion optic supply board are listed in Table 2-5. The positions of the diagnostic LEDs on the board are indicated by white rectangles in Figure 2-34.

Table 2-5. Diagnostic LEDs on the ETD Ion Optic Supply board

No.	Name	Color	Description	Normal Operating Condition
LD1	+275 V	Green	+275 V input voltage present	On
LD2	-275 V	Green	-275 V input voltage present	On
LD3	RF Supply	Green	RF input voltage (22 V) present	On
LD4	+24 V	Green	+24 V input voltage present	On
LD5	+15 V	Green	+15 V input voltage present	On
LD6	-15 V	Green	-15 V input voltage present	On
LD7	RF1_ON	Blue	RF-generator switched on	On/Off, depending on active application

Preamplifier

The preamplifier is located in a housing next to the Cold Ion Gauge. See Figure 2-34. It is water cooled to protect it during a system bakeout.

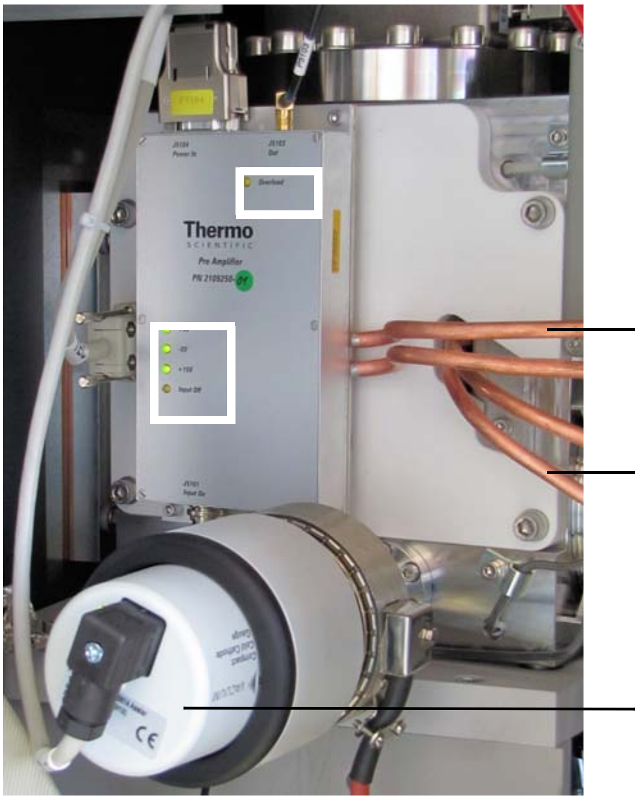


Figure 2-34. Preamplifier

This board is a broadband preamplifier with differential high-impedance inputs. It serves as a detection amplifier and impedance converter for the image current created by the oscillating ions. The output current is transferred to the data acquisition board. It has an amplification factor of about 60 dB and covers the frequency range from 15 kHz to 10 MHz.

The diagnostic LEDs on the preamplifier are listed in Table 2-6. The positions of the diagnostic LEDs on the board are indicated by white rectangles in Figure 2-34.

Table 2-6. Diagnostic LEDs on the Preamplifier board

No.	Name	Color	Description	Normal Operating Condition
LD1	Overload	Yellow	RF output is overloaded	Off
LD2	+5 V	Green	+5 V input voltage present	On
LD3	+15 V	Green	+15 V input voltage present	On
LD4	-5 V	Green	-5 V input voltage present	On
LD5	Input off	Yellow	RF inputs are shortened (protection)	On, off during Detect

Internal Computer

Figure 2-35 shows the components of the data acquisition unit. The unit is mounted in a housing at the right side of the instrument.

Figure 2-35. Data Acquisition unit

The internal computer contains a computer mainboard with an ATX power supply. The data acquisition digital PCI board is directly plugged into the mainboard. The data acquisition analog board is mounted on top of the computer mainboard.

Data Acquisition Digital PCI Board

Figure 2-36 shows the data acquisition digital PCI board. It is an add-on board to the internal computer. (See Figure 2-35 on page 2-48.)

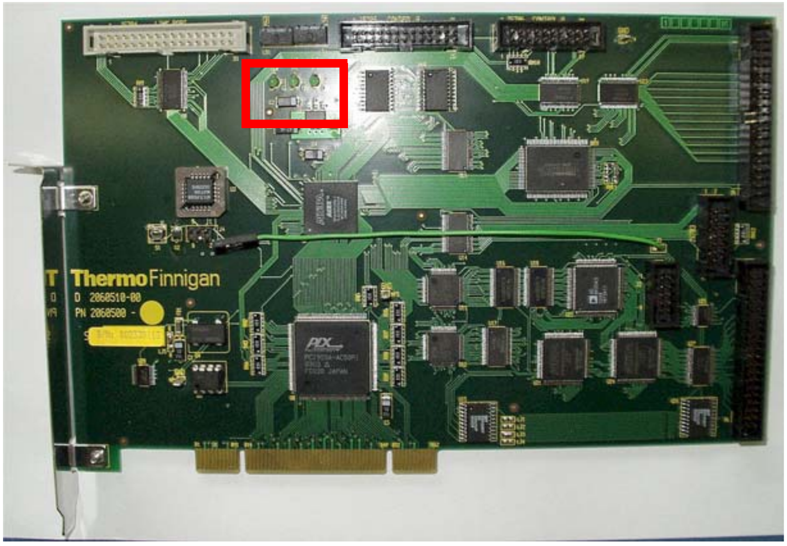


Figure 2-36. Data Acquisition Digital PCI board

This board is used to convert detected ion signals to digital form and to interface to the computer mainboard. The board has two 16 bit parallel connections to the DAC and the ADC on the data acquisition analog board, which are used for controlling and reading-back signals. A high-speed link port channel is also on the board that is used to communicate with the electronics in the linear ion trap.

Precision timing is derived from the data acquisition analog board and events with lower requirements use the timer in the internal computer. This timer is used to check at regular intervals whether the foreground process works as expected.

Communication takes place not only between the linear ion trap and the internal computer of the Orbitrap Elite system, but also between the linear ion trap and the data system computer. For further information about the data system, refer to the *LTQ Series Hardware Manual.*

The diagnostic LEDs listed in Table 2-7 show the status of the board. The position of the LEDs on the board is indicated by a red rectangle in Figure 2-36.

Table 2-7. Diagnostic LEDs of the Data Acquisition Digital PCI board

Name	Color	Description	Normal Operating Condition
+5 V	Green	+5 V voltage present	On
+3.3 V	Green	+3.3 V voltage present	On
+2.5 V	Green	+2.5 V voltage present	On

Data Acquisition Analog Board

Figure 2-37 shows the data acquisition analog board. This board is an add-on board to the mainboard of the internal computer. See Figure 2-35 on page 2-48. It is used to convert analog to digital signals for Orbitrap analyzer experiments, especially for detecting the ions. The board contains an ADC for the detection of the transient signal, with a frequency range from 10 kHz to 10 MHz. Three anti-aliasing filters for the low, middle and high mass range are automatically selected by the software.

The data acquisition board provides precision timing to control the acquisition. Events with lower timing requirements on accuracy are controlled by the linear ion trap.

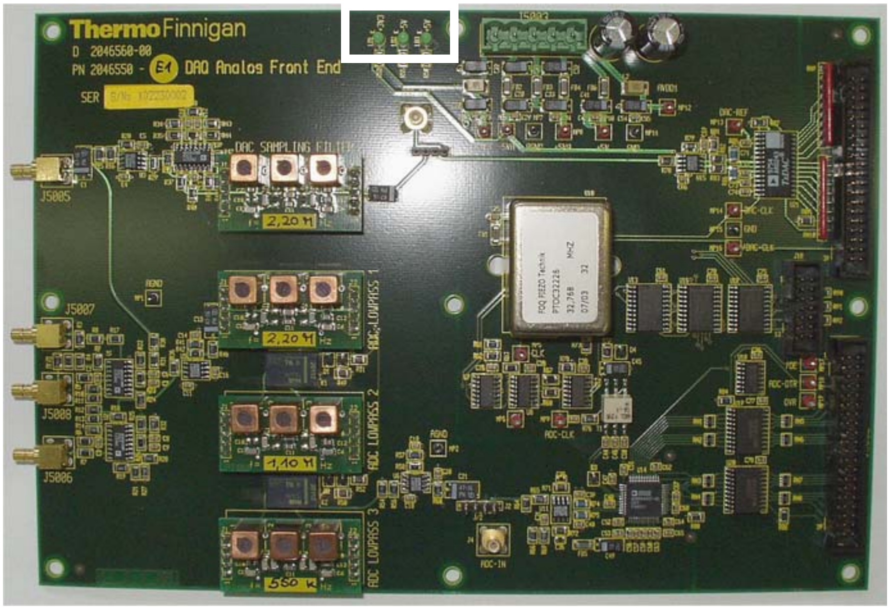


Figure 2-37. Data Acquisition Analog board

The diagnostic LEDs listed in Table 2-8 show the status of the voltages applied to the board. The position of the LEDs on the board is indicated by a white rectangle in Figure 2-37.

Table 2-8. Diagnostic LEDs of the Data Acquisition Analog board

Name	Color	Description	Normal Operating Condition
+5 V	Green	+5 V voltage present	On
-5 V	Green	-5 V voltage present	On
+3.3 V	Green	+3.3 V voltage present	On

Power Supply 2 Board

The power supply 2 board provides the supply voltages for the data acquisition analog board. It is mounted to the back inside the housing of the internal computer. See Figure 2-35 on page 2-48.

The diagnostic LEDs listed in Table 2-9 show the status of the voltages applied to the board.

Table 2-9. Diagnostic LEDs of the Power Supply 2 board

Name	Color	Description	Normal Operating Condition
+5.1 V	Green	+5.1 V voltage present	On
-5.1 V	Green	-5.1 V voltage present	On
+3.3 V	Green	+3.3 V voltage present	On

Instrument Control Board

Figure 2-38 shows the instrument control board. The instrument control board is in a housing next to the internal computer. It is connected to the Orbitrap Elite MS main power.

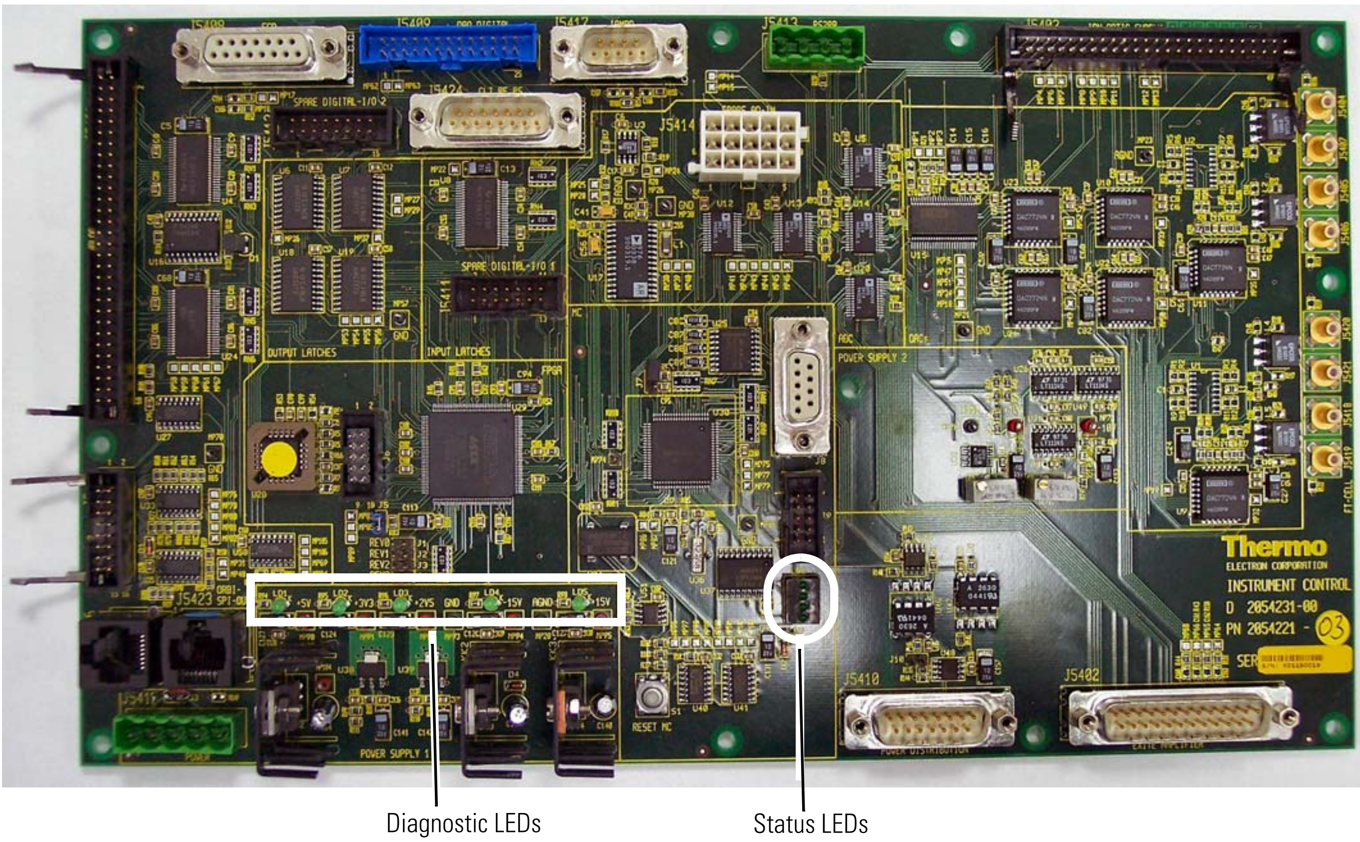


Figure 2-38. Instrument Control board

The instrument control board is used to interface the Velos Pro MS control electronics to the Orbitrap analyzer control electronics. Three signal lines are passed from the Velos Pro MS: a digital, parallel (DAC) bus, a serial SPI bus, and a Link Port Signal line. The instrument control board contains a micro controller, digital and analog converters, and serial port connectors.

On the instrument control board, analog signals from vacuum gauges are converted to digital signals and passed to the data system as well as to the power distribution board. (See page 2-52.) Turbomolecular pumps (See "Vacuum System" on page 2-30.) are attached to a serial port connector and this is connected via the signal lines to the linear ion trap.

The diagnostic LEDs listed in Table 2-10 show the status of applied voltages to the board. The position of the diagnostic LEDs on the board is indicated by a white rectangle in Figure 2-38 on page 2-51.

Table 2-10. Diagnostic LEDs of the Instrument Control board

No.	Name	Color	Description	Normal Operating Condition
LD1	2.5 V	Green	2.55 V Input voltage present	On
LD2	3.3 V	Green	3.3 V Input voltage present	On
LD3	5 V	Green	5 V Input voltage present	On
LD4	-15 V	Green	-15 V Input voltage present	On
LD5	+15 V	Green	+15 V Input voltage present	On

Additionally, the board has four green LEDs that are directly connected to the micro controller. They indicate the state of the micro controller and possible error bits and can be used for software debugging. See Table 2-11. The position of the status LEDs on the board is indicated by a white oval in Figure 2-38 on page 2-51.

Table 2-11. Software status LEDs of the Instrument Control board

No.	Description	Normal Operating Condition
6.1	Micro controller is working properly	Permanent flashing of LED
6.2	CAN bus connection to power distribution board enabled	On
6.3	Connection to internal computer and Velos Pro SPI bus enabled	On
6.4	Orbitrap analyzer SPI bus enabled	On Flashing on error

Power Distribution Board

Figure 2-39 shows the power distribution board. It is located at the bottom of the right side of the instrument. The power distribution board controls the vacuum system and the system power supplies, including the linear ion trap. Depending on the quality of the vacuum and the status of the turbo molecular pumps, it switches the vacuum gauges, the pumps, and the 230 V relays. It controls external relays with 24 V DC connections. In case of a vacuum failure, it initiates an automatic power down of the instrument.

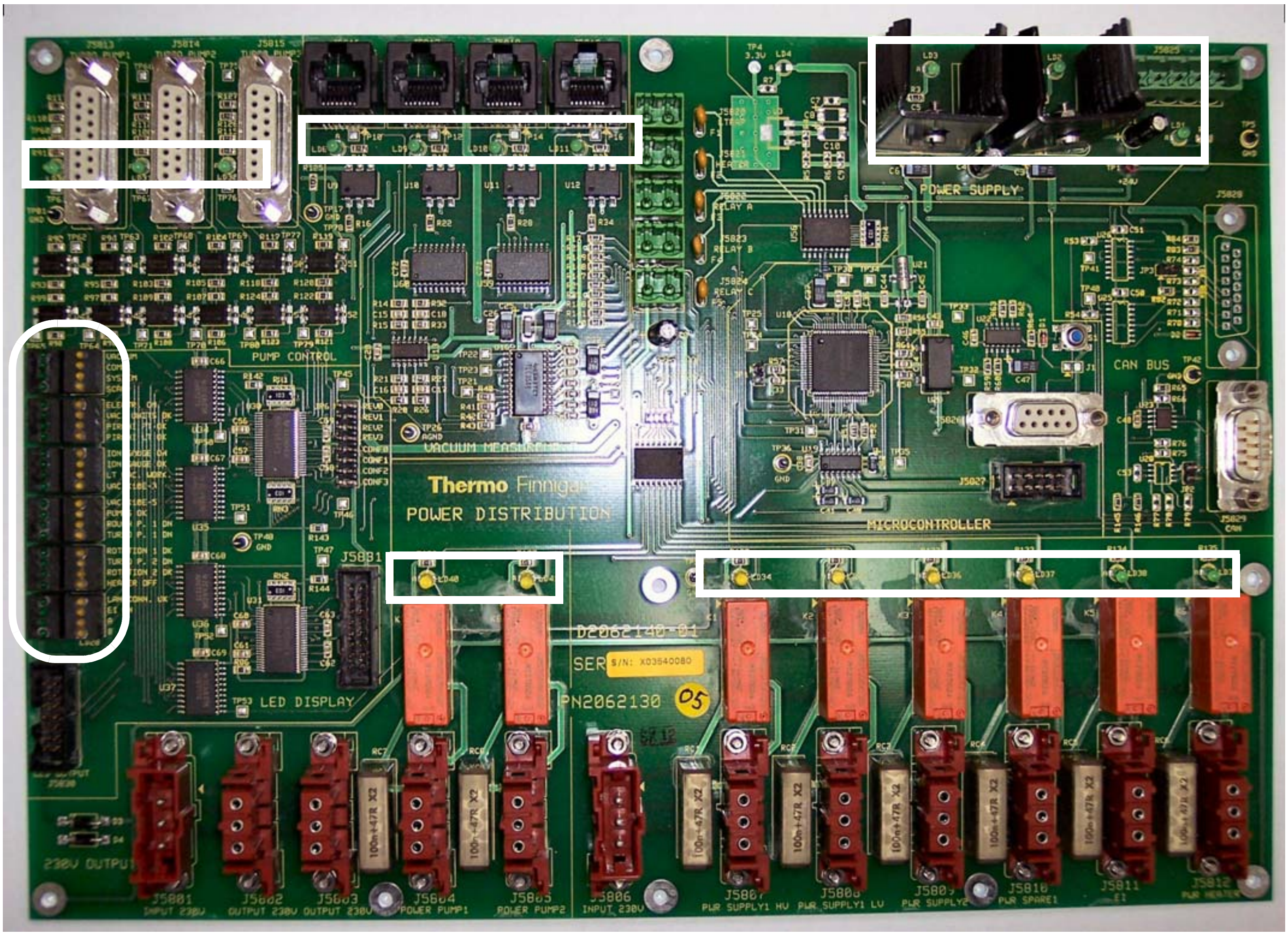


Figure 2-39. Power Distribution board

The power distribution board indicates all system states and error messages by status LEDs (See Table 2-12 on page 2-54.) in the middle of the left side of the board. A green LED indicates that the status is OK. An orange LED indicates a status that differs from normal. The position of the LEDs on the board is indicated by a white oval in Figure 2-39.

The system status LEDs on the front side of the instrument (See Figure 2-4 on page 2-5.) are controlled by the power distribution board. The information partially comes from external boards (for example, the Communication LED is controlled by the instrument control board). (See “Instrument Control Board” on page 2-51.)

Diagnostic LEDs show the status of voltages applied from the board to other devices. The positions of the diagnostic LEDs on the board are indicated by white rectangles in Figure 2-39.

Table 2-12. Status LEDs of the Power Distribution board

LED green	LED orange	Information given by orange LED
Vacuum	High vacuum failure	High vacuum pressure > 10^{-8} mbar
Comm.	No communication with instrument control board	CAN bus problem or instrument control board not working
System	System is not ready	FT Electronics switch off or Vacuum Pumps switch off
Scan		Instrument is not scanning
Electr. On	Service mode	FT Electronics switch off
Vac. Units OK	Vacuum measurement failure	Vacuum gauge defective
Pirani Orbitrap analyzer OK	No function, at present	
Pirani LT OK	Pirani Velos Pro MS failure	Control signal < 0.5 V
Ion Gauge On	Penning Orbitrap Elite MS Off	Forevacuum > 10^{-2} mbar
Ion Gauge OK	Penning Orbitrap Elite MS failure	Control signal < 0.5 V
LT Vacuum Work	Velos Pro MS vacuum failure	Vacuum forepump Velos Pro MS >10^{-1} mbar
Vac. <10^{-3}	Forevacuum failure	Forevacuum > 10^{-3} mbar
Vac. <10^{-5}	High vacuum failure	High vacuum > 10^{-5} mbar
Pumps OK	Pumps Off	Pump down; leakage
Rough P. 1 On	Forepump #1 failure	Forepump defective
Turbo P. 1 On	TMP 1 failure	TMP defective/error[a]
Rotation 1 OK	TMP 1 failure	80% rotation speed of TMP not reached
Turbo P. 2 On	TMP 2 failure	TMP defective/error[a]
Rotation 2 OK	TMP 2 failure	80% rotation speed of TMP not reached
Heater Off	Heater enabled	Heater enabled
LAN Conn. OK	LAN connection failure	LAN interrupted (Option)
EI On	No function, at present	
A	System reset	System reset has occurred
B		Micro controller idle

[a] An error of TMP 3 is indicated by an LED directly on the pump controller. An error of TMP 4 is indicated in the software.

Depending on user actions, the power distribution is switched to various working modes by the hardware. See Table 2-13.

Table 2-13. Working modes of the Power Distribution board

	Action	Consequences
a.	Main switch off	Complete system including linear ion trap and multiple socket outlets (ETD Module, for example) are without power
b.	Vacuum Pumps switch off	Everything is switched off
c.	FT Electronics switch off	All components are switched off with exception of the following ones: • Heater control • Multiple socket outlets • Power distribution board • Pumps • Vacuum control • Velos Pro MS (has a separate Service switch)

Table 2-14 shows the possible operating states of the power distribution.

Table 2-14. Operating states of the Power Distribution board

	Action	Consequences
1.	Main switch on, Vacuum Pumps switch off	Everything is switched off
2.	Vacuum Pumps switch on and FT Electronics switch on	System starts up: pumps and electronics switched on
3.	Check linear ion trap and Orbitrap Elite MS forevacuum pumps: 10^{-0} mbar after 30 s.	If not ok: switch off system and light error LED[a]; power distribution remains switched on
4.	After the system has started, the Pirani gauge returns a vacuum < 10^{-2} mbar and both TMPs reach 80% rotation speed	Switch on Penning gauge
5.	Vacuum and 80% rotation speed of TMPs not reached after preset time (< 8 min, otherwise the pumps automatically switch off).	Switch off system (including linear ion trap) and light error LED*; power distribution remains switched on
6.	One or more vacuum gauges defective (control signal < 0.5 V).	Light error LED only, otherwise ignore
7.	After the operating status is reached, the pressure at one gauge exceeds the security threshold for more than the preset time period: • Pirani gauge Orbitrap Elite MS >10^{-1} mbar • Penning gauge Orbitrap Elite MS >10^{-3} mbar • Pirani gauge Velos Pro MS forepump >10^{-1} mbar	System is shut down with exception of power distribution (light error LED). Rebooting of the system by switching off/on of the main switch.
8.	Rotation speed of a TMP falls below 80%	Shut down system (see 7.); light LED* of corresponding pump.

Table 2-14. Operating states of the Power Distribution board, continued

	Action	Consequences
9.	Service switch linear ion trap off	Linear ion trap electronics switched off, pumps keep on running; Orbitrap Elite MS without data link, keeps on running
10.	FT Electronics switch Orbitrap Elite MS off	Orbitrap Elite MS electronics switched off, pumps keep on running; Orbitrap Elite MS without data link, keeps on running
11.	Failure of linear ion trap or Orbitrap Elite MS (for example, fuse is opened).	If the vacuum in one part deteriorates, the complete system is shut down.
12.	Mains failure	System powers up after the electricity is available again. All devices reach the defined state. Linear ion trap and internal computer must reboot.

[a] After the shutdown, the LED flashes that represents the reason for the shutdown.

Power Supply 1 Board

Figure 2-40 shows the power supply 1 board. This board is next to the power distribution board. It provides the power for the ion optic supply board (See "Ion Optic Supply Board" on page 2-58.) and the instrument control board. (See "Instrument Control Board" on page 2-51.)

Figure 2-40. Power Supply 1 board

The diagnostic LEDs listed in Table 2-15 show the status of the voltages applied to the board. The position of the LEDs on the board is indicated by the white rectangles in Figure 2-40.

Table 2-15. Diagnostic LEDs of the Power Supply 1 board

Name	Color	Description	Normal Operating Condition
+285 V	Green	+285 V Output voltage present	On
-285 V	Green	-285 V Output voltage present	On
Over Current +285 V	Red	LED lit dark red: I_{out} > 80 mA LED lit bright red: output is short-circuited	Off
Over Current -285 V	Red	LED lit dark red: I_{out} > 80 mA LED lit bright red: output is short-circuited	Off
+18 V	Green	+18 V Output voltage present	On
-18 V	Green	-18 V Output voltage present	On
+8.5 V	Green	+8.5 V Output voltage present	On

Electronic Boards on the Left Side of the Instrument

Figure 2-41 shows the left side of the instrument with the panel opened. This side of the instrument contains mostly boards that are part of the Orbitrap analyzer control.

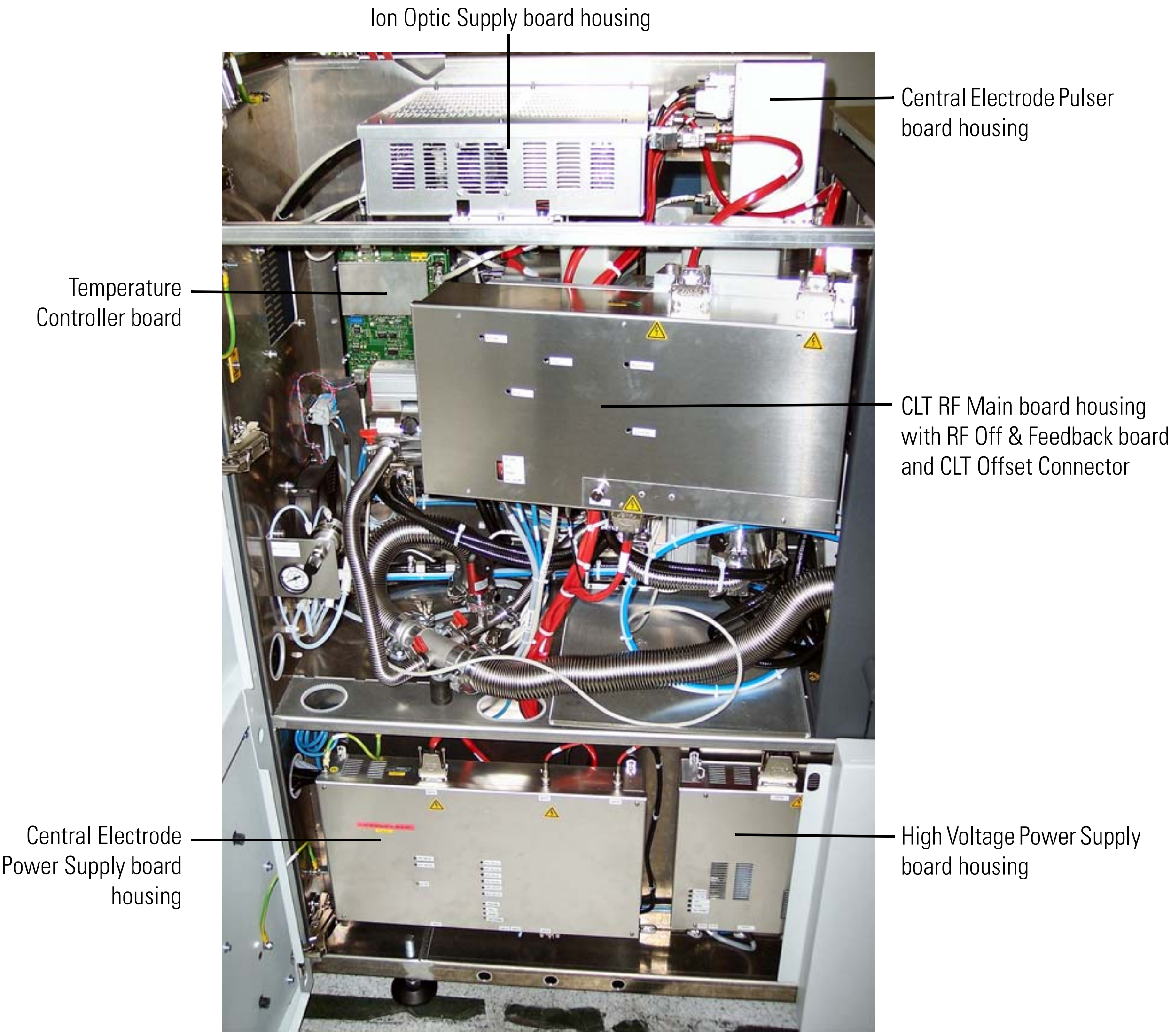


Figure 2-41. Electronic boards on the left side of the instrument

The main components on this side are described starting from the top.

Ion Optic Supply Board

Figure 2-42 shows the ion optic supply board. The board is in a housing on top of the left instrument side of the instrument. This board supplies the voltages and the radio frequency for the ion guides and interoctapole lenses of the Orbitrap Elite mass spectrometer. It has an RF detector for the RF output control. The board also provides the trap voltage, the gate voltage, and the reflector DC voltages as well as the RF voltages to the octapole of the Orbitrap analyzer. See "Orbitrap Analyzer" on page 2-14 for further information.

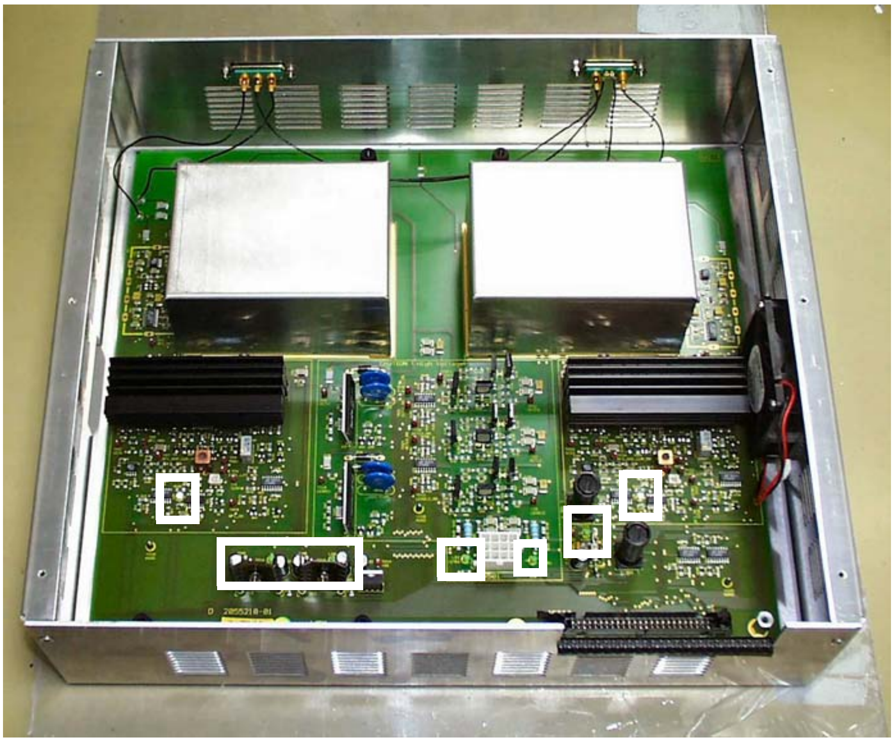


Figure 2-42. Ion Optic Supply board

The diagnostic LEDs listed in Table 2-16 show the status of applied voltages to the board. The position of the LEDs on the board is indicated by white rectangles in Figure 2-42.

Table 2-16. Diagnostic LEDs of the Ion Optic Supply board

No.	Name	Color	Description	Normal Operating Condition
LD1	+275 V	Green	+275 V Input voltage present	On
LD2	-275 V	Green	-275 V Input voltage present	On
LD3	+29 V	Green	+29 V Input voltage present	On
LD5	+15 V	Green	+15 V Input voltage present	On
LD6	-15 V	Green	-15 V Input voltage present	On
LD7	RF1_ON	Blue	RF1 generator switched on	depending on application; LED flashes during scanning
LD8	RF2_ON	Blue	RF2 generator switched on	depending on application; LED flashes during scanning

Central Electrode Pulser Board

The central electrode pulser board is located in a housing that is mounted to the flange of the UHV chamber. See Figure 2-43.

Figure 2-43. Central Electrode Pulser board

The board switches the injection and measurement voltages for the central electrode and the detection electrodes of the Orbitrap analyzer. Resistor-capacitor circuits on the board convert the switching pulse into a smooth transition between the voltages.

The diagnostic LEDs listed in Table 2-17 show the status of the voltages applied to the board as well as some operating states. The position of the LEDs on the board is indicated by the white rectangles in Figure 2-43.

Table 2-17. Diagnostic LEDs of the Central Electrode Pulser board

No.	Name	Color	Description	Normal Operating Condition
LD1	TRIG	Green	Trigger signal indicator	Flashing when scanning
LD2	PS	Green	24 V Power Supply is OK	On

Temperature Controller Board

The temperature controller board is on the top left side of the instrument, next to the CLT RF main board. See Figure 2-41 on page 2-58. The temperature controller board keeps the temperature of the analyzer chamber to a preset value. A Peltier element that can be used for heating as well as for cooling is used as an actuator. Activation is done via the serial SPI (Serial Peripheral Interface) bus.

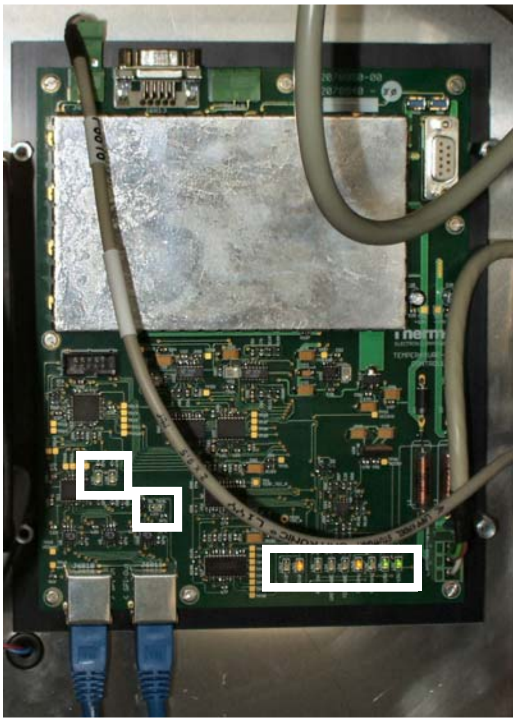


Figure 2-44. Temperature Controller board

The diagnostic LEDs listed in Table 2-18 show the status of the voltages applied to the board as well as some operating states. The positions of the LEDs on the board are indicated by the white rectangles in Figure 2-44.

Table 2-18. Diagnostic LEDs of the Temperature Controller board

No.	Name	Color	Description	Normal Operating Condition
LD1	+15 V	Green	+15 V Input voltage present	On
LD2	-15 V	Green	-15 V Input voltage present	On
LD3	TEC >60C	Yellow	Temperature of cold side Peltier element above 60 °C	Off
LD4	Unit >60C	Yellow	Temperature of UNIT heat sink above 60 °C	Off
LD5	Reg Off	Yellow	Control switched off	Off
LD6	No Term	Yellow	SPI bus termination board missing	Off
LD7	SDT enable	Green	Interface has been addressed and sends/receives data	Flashing on SPI bus data transfer
LD8	SEL	Green	Board has been addressed	Flashing on SPI bus data transfer
LD9	Heating	Yellow	Peltier element is heating	Depending on system state
LD10	Cooling	Yellow	Peltier element is cooling	Depending on system state
LD11	UR>0	Yellow	Summation voltage controller >0 V	Off when adjusted
LD12	UR<0	Yellow	Summation voltage controller <0 V	Off when adjusted

CLT RF Unit

The CLT RF unit comprises the CLT RF main board and the RF off & feedback board. The unit operates the curved linear trap (CLT) with four phases RF voltage and three pulsed DC voltages (PUSH, PULL, and OFFSET).

The CLT RF main board is located in a housing in the center of the left side of the instrument. See Figure 2-41 on page 2-58. This board provides an RF voltage ("Main RF") for the curved linear trap. It allows switching off the RF and simultaneous pulsing of each CLT electrode. See "Orbitrap Analyzer" on page 2-14 for further information. The board communicates with the instrument control board via an SPI bus.

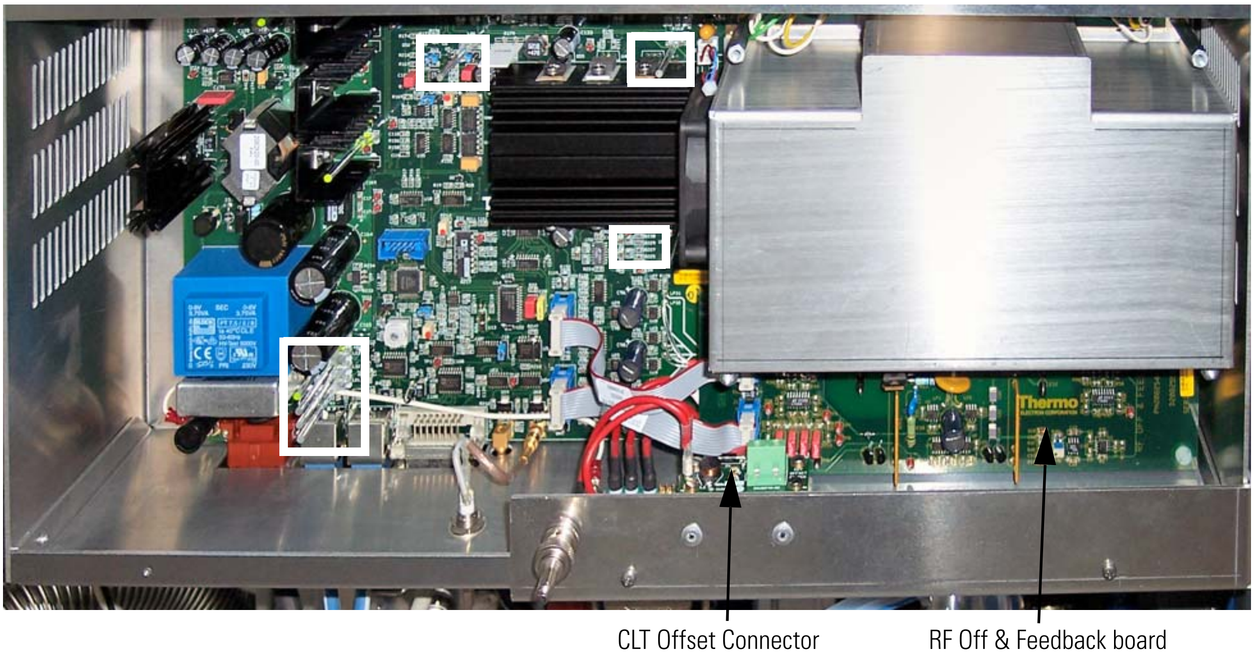


Figure 2-45. CLT RF unit (cover removed)

The diagnostic LEDs listed in Table 2-19 show the status of the voltages applied to the board as well as some operating states. The position of the LEDs on the board is indicated by the white rectangles in Figure 2-45.

Table 2-19. Diagnostic LEDs of the CLT RF Main board

No.	Name	Color	Description	Normal Operating Condition
LD1	NO TERM	Yellow	SPI bus termination board missing	Off
LD2	SEND	Yellow	Interface has been addressed and sends/receives data	Flashing on SPI bus data transfer
LD3	SEL	Green	Board has been addressed	Flashing on SPI bus data transfer
LD4	RF ON	Green	RF voltage on	On
LD5	NO LOCK	Yellow	PLL has been not locked	50% intensity

Table 2-19. Diagnostic LEDs of the CLT RF Main board, continued

No.	Name	Color	Description	Normal Operating Condition
LD6	OVL	Yellow	RF Amplifier overload	Off
LD7	OVHEAT	Red	Heatsink temperature > 73 °C	Off

The RF off & feedback board is an add-on board to the CLT RF main board. It is located in the same housing. See Figure 2-45.

The CLT Offset connector, which removes interfering signals from the circuit, is also mounted in the housing.

Central Electrode Power Supply Board

The central electrode power supply board is mounted in a housing on the bottom left side of the instrument. See Figure 2-46.

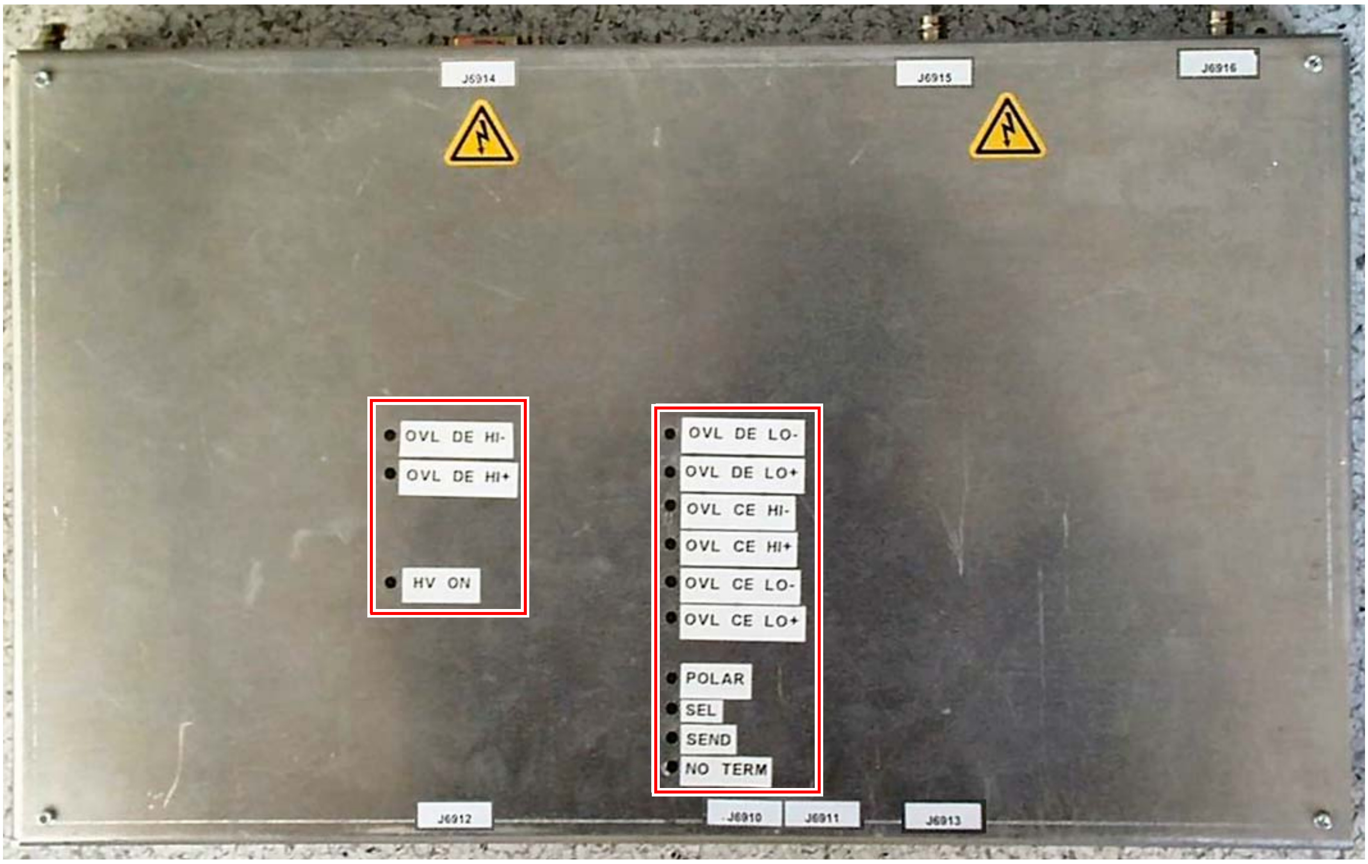


Figure 2-46. Central Electrode Power Supply board

The board supplies four DC voltages to the Orbitrap analyzer:

- Two central electrode (CE) voltages: CE HIGH 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 3 kV and the maximum DE voltage is 1 kV. The board communicates via the SPI bus.

In addition to a ventilator on the bottom right side, a water-cooled Peltier element on the rear side of the board serves as means of heat dissipation.

The diagnostic LEDs listed in Table 2-20 show the status of the voltages applied to the board as well as some operating states. The position of the LEDs on the board is indicated by the red rectangles in Figure 2-46 on page 2-63.

Table 2-20. Diagnostic LEDs of the Central Electrode Power Supply board

No.	Name	Color	Description	Normal Operating Condition
LD1	OVL DE HI-	Yellow	Negative side of Deflector High Supply has been overloaded	Off when HV is switched on
LD2	OVL DE HI+	Yellow	Positive side of Deflector High Supply has been overloaded	Off when HV is switched on
LD3	No Term	Red	SPI bus termination board missing	Off
LD4	Send	Yellow	Interface has been addressed and sends/receives data	Flashing on SPI bus data transfer
LD5	Sel	Green	Board has been addressed	Flashing on SPI bus data transfer
LD6	Polarity	Blue	Positive/negative ion mode	Off (positive mode)
LD7	OVL CE LO+	Yellow	Positive side of Central Electrode Low Supply has been overloaded	Off when HV is switched on
LD8	OVL CE LO-	Yellow	Negative side of Central Electrode Low Supply has been overloaded	Off when HV is switched on
LD9	OVL CE HI+	Yellow	Positive side of Central Electrode High Supply has been overloaded	Off when HV is switched on
LD10	OVL CE HI-	Yellow	Negative side of Central Electrode High Supply has been overloaded	Off when HV is switched on
LD11	OVL DE LO+	Yellow	Positive side of Deflector Low Supply has been overloaded	Off when HV is switched on
LD12	OVL DE LO-	Yellow	Negative side of Deflector Low Supply has been overloaded	Off when HV is switched on
LD13	HV ON	Green	High voltage switched on	On when HV is switched on

High Voltage Power Supply Board

The high voltage power supply board is mounted in a housing on the bottom left side of the instrument. See Figure 2-41 on page 2-58. This board provides five DC voltages for the ion optics of the Orbitrap Elite mass spectrometer. Two voltages supply the lenses of the instrument. Three voltages are applied to the RF CLT main board to be used as focusing potentials for the curved linear trap. See "Orbitrap Analyzer" on page 2-14 for further information. The board communicates via the SPI bus.

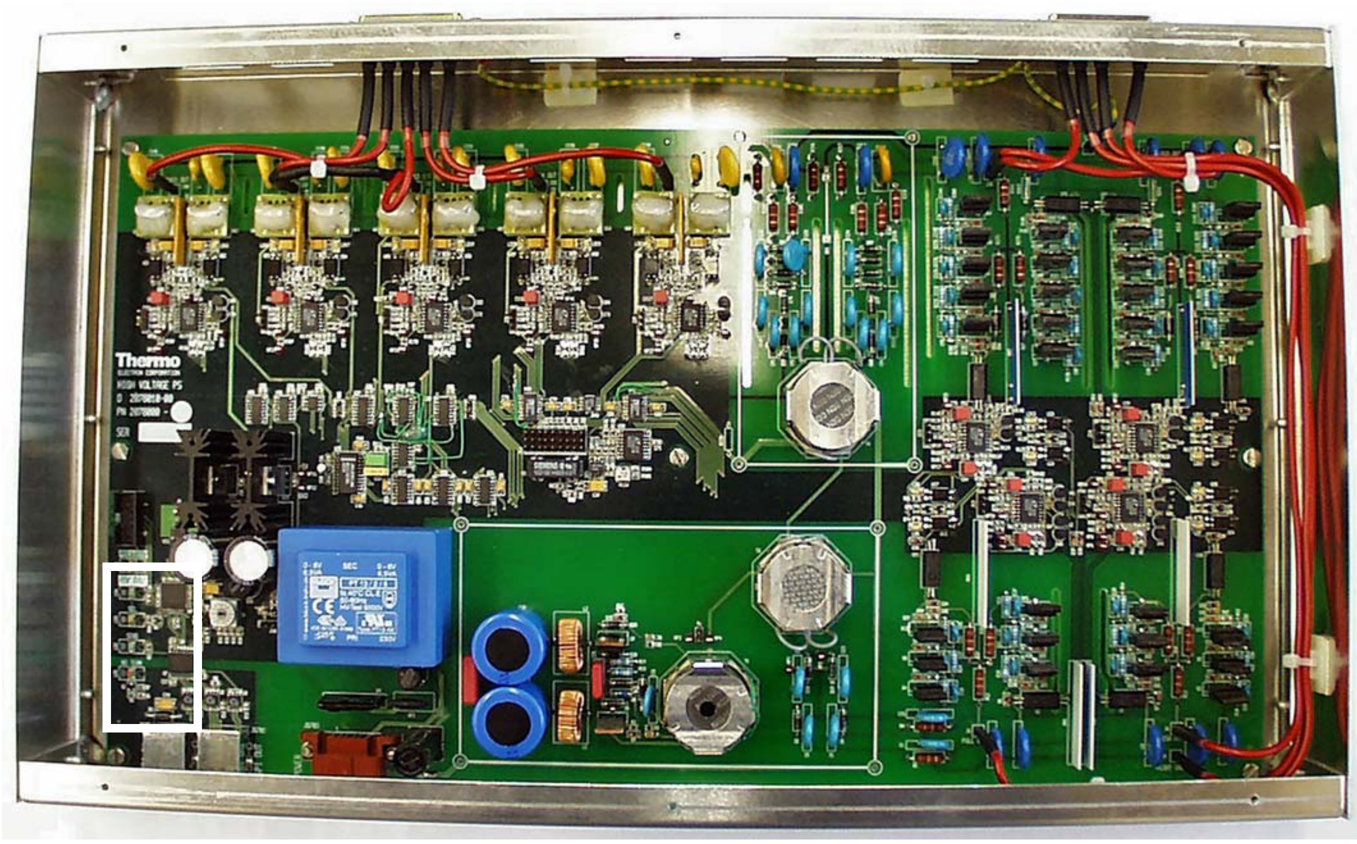


Figure 2-47. High Voltage Power Supply board (cover removed)

The diagnostic LEDs listed in Table 2-21 show the operating states of the board. The position of the LEDs on the board is indicated by the white rectangles in Figure 2-47.

Table 2-21. Diagnostic LEDs of the High Voltage Power Supply board

No.	Name	Color	Description	Normal Operating Condition
LD1	NO TERM	Red	SPI bus termination board missing	Off
LD2	SEND	Yellow	Interface has been addressed and sends/receives data	Flashing on SPI bus data transfer
LD3	SEL	Green	Board has been addressed	Flashing on SPI bus data transfer
LD4	HV ON	Green	High voltage is switched on	On
LD5	POLARITY	Green	Positive/negative ion mode	Off (positive mode)

SPI Bus Termination Board

Various boards communicate via the SPI bus, a serial RS485-based bus system. The SPI Bus Termination board reduces unwanted signal reflections. The boards indicate a missing termination (after maintenance, for example) by LEDs.

The SPI Bus Termination board is located below the High Voltage Power Supply board, at the bottom left side of the instrument. See Figure 2-48.

Figure 2-48. High Voltage Power Supply board with SPI Bus Termination board

Chapter 3 Safety

This chapter contains information that is important for your own safety or the safety of others, and that prevents damage to the instrument, Read this chapter carefully before you install or operate the instrument and its accessories, or come into contact with it.

Contents

Safety Symbols and Signal Words in this Manual

Notices concerning the safety of the personnel operating the Orbitrap Elite 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.

Rating Plate

To identify correctly the instrument when you contact Thermo Fisher Scientific, always have the information from the rating plate available. It contains the serial number, which is important in any type of communication with Thermo Fisher Scientific.

The rating plate of Orbitrap Elite MS is attached to the top left corner of the rear side of the instrument. The rating plate of the Orbitrap Elite ETD MS is attached to the right side of the bottom panel of the ETD Module.

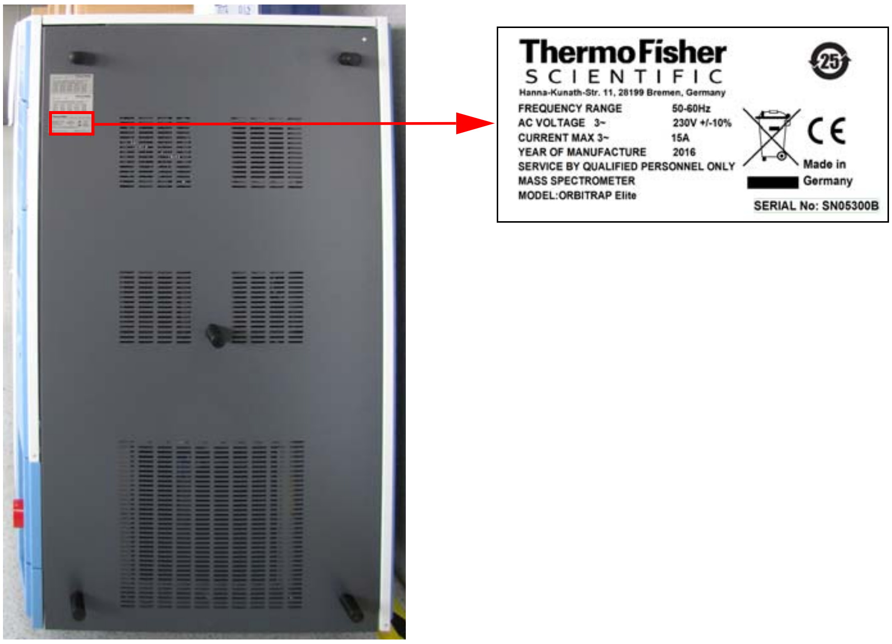


Figure 3-1. Orbitrap Elite MS rating plate

Figure 3-2. Orbitrap Elite ETD MS rating plate

Note that the ETD Module itself also has a rating plate. It is located in the bottom left corner of the ETD Module.

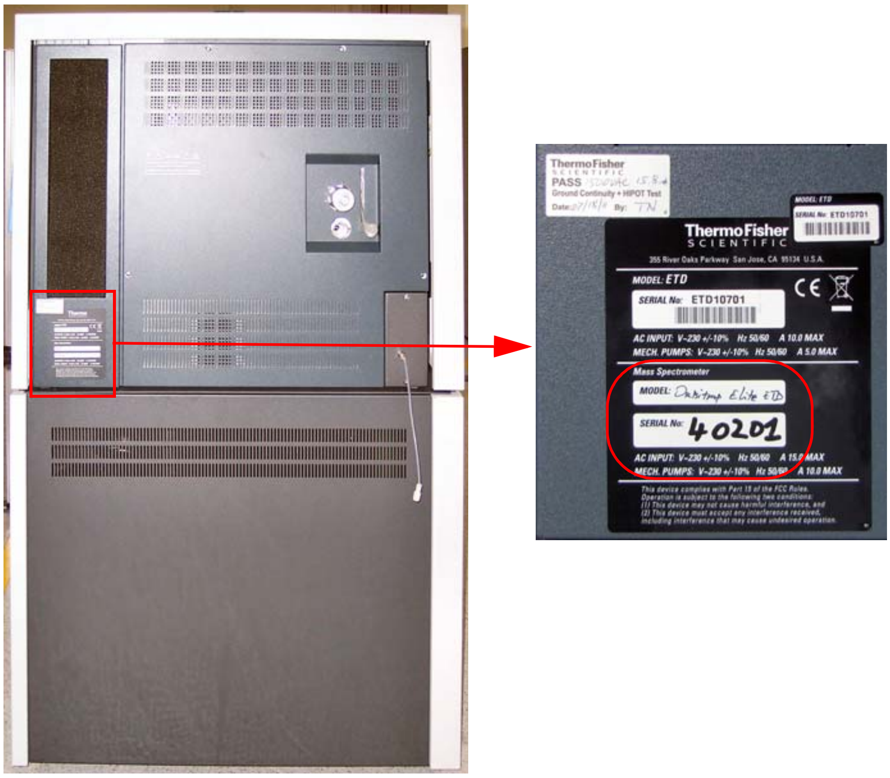


Figure 3-3. ETD Module rating plate

Intended Use

The Orbitrap Elite mass spectrometer is a a hybrid mass spectrometer comprising a dual cell linear ion trap and an Orbitrap analyzer with new geometry and improved signal processing. It is used for liquid chromatography (LC) mass spectrometry (MS) high throughput applications.

⚠ Observe the following usage guidelines when you operate your Orbitrap Elite mass spectrometer:

- The instrument is designed to be operated under carefully controlled conditions. It is not designed for the use outdoors.
- The instrument is designed to be used exclusively with API sources and probes approved 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 Orbitrap Elite 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 API sources and probes.

Qualification of the Personnel

⚠ Only employees of Thermo Fisher Scientific or personnel acting on behalf of Thermo Fisher Scientific are allowed to install the Orbitrap Elite mass spectrometer.

Personnel that install or operate Orbitrap Elite MS 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, PE connection). Refer to the *LTQ Orbitrap Series Preinstallation Requirements Guide* for the specifications.

- General Operation

  The Orbitrap Elite MS is 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

The Orbitrap Elite mass spectrometer is designed to be operated with the following materials:

- Nitrogen gas: Used for the API sheath gas, API auxiliary/sweep gas, C-Trap bath gas, and HCD collision gas. Also used as reagent carrier gas in the ETD Module.
- Helium gas: Used for the collision gas of the linear trap
- Forepump oil: Used for cooling, lubrication, and sealing of the forepump

  NOTICE Use only the forepump oil indicated on the name plate and pump. If other oils are used, the manufacturer rejects all responsibility should any trouble occur. ▲

- Calibration compounds, samples
- Solvents
- Fluoranthene: Used as Electron Transfer Dissociation (ETD) reagent in the ETD Module portion of the Orbitrap Elite ETD mass spectrometer

For information about the material permitted to operate the API source, refer to the *Ion Max and Ion Max-S API Source Hardware Manual*.

Electric Safety Precautions

⚠ **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:

- Do not change the external or internal grounding connections. Tampering with or disconnecting these connections could endanger you and/or damage the system.
- 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.
- Do not run the system without the housing on. Permanent damage can occur. When you leave 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 switch on the instrument if you suspect that it has incurred any kind of electrical damage. Instead, disconnect the power cord of the mass spectrometer and contact a Thermo Fisher Scientific field service engineer for a product evaluation. Do use the instrument until it has been evaluated. Electrical damage might have occurred if the system shows visible signs of damage, or has been transported under severe stress.
- Do not place any objects upon 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

If you need to switch off the mass spectrometer in an emergency, place the main power switch (located on the power panel at the right side of the Orbitrap Elite MS) in the Off (0) position. This switches off all power to the instrument, including the linear ion trap, multiple socket outlets, and the vacuum pumps. The main power switch must be turned 90° counterclockwise to switch off the instrument. See Figure 3-4.

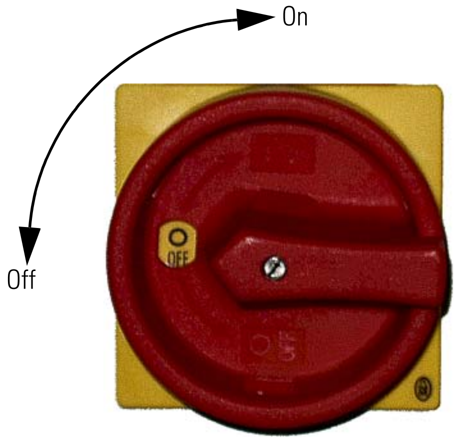


Figure 3-4. Main power switch in Off position

The instrument is automatically vented by the vent valve of the linear ion trap. The vent valve vents the system 30 seconds after power is switched off.

Although removing power abruptly will not harm any component within the system, this is not the recommended shutdown procedure to follow. See "Shutting Down the Instrument" on page 5-7 for the recommended procedure.

⚠ WARNING **Electric Current.** Electric shock hazard. Capacitors inside the instrument might still be charged even if the instrument is switched off. Wait for sufficient time before you remove the instrument housing.

To separately switch off the recirculating chiller or the computer in an emergency, use the On/Off switches on the chiller and computer, respectively.

Behavior of the System in Case of a Main Failure

A main power failure has the same consequence as switching off with the main power switch. If the power is available again, the system starts up automatically: the pumps are switched on and the instrument is pumped down. 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 6-6.

It is not possible to check whether the system was vented. The log file of the data system indicates a reboot of the system. 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.

NOTICE The intentional venting of the system is performed with the vent valve of the linear ion trap. ▲

Residual Hazards

Users of the Orbitrap Elite mass spectrometer must pay attention to the following residual hazards.

⚠ WARNING **High Voltage.** If you touch liquid leaking from the probe sample inlet while the mass spectrometer is in operation, you might receive an electric shock. Do not tighten the probe sample inlet fitting to eliminate a liquid leak while the mass spectrometer is in operation.

⚠ WARNING **Hazardous Chemicals.** The effluent of the forepumps might contain noxious chemicals. The forepumps eventually exhaust much of what is introduced into the mass spectrometer, including the small amount of oil vapor that mechanical pumps can emit. The connection to an adequate exhaust system is mandatory!

⚠ WARNING **Suffocation Hazard.** Accumulation of nitrogen gas could displace sufficient oxygen to suffocate personnel in the laboratory. Most of the nitrogen that is introduced into the API source (about 5000 L or 180 ft^3 per day) escapes into the laboratory atmosphere. Ensure that the laboratory is well ventilated. Always operate Orbitrap Elite mass spectrometer and API source with attached drain tubing assembly that connects the source housing drain to a dedicated exhaust system.

⚠ 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 cord of the mass spectrometer before you try any type of maintenance.

⚠ 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. Forepump in function is hot and some surfaces could reach a temperature higher than 80 °C (176 °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, ion transfer capillary and sweep cone might reach temperatures of up to 450 °C. To cool the ion transfer capillary, set the capillary temperature to 25 °C or place the electronics service switch in the Service Mode position. Wait until the ion source has cooled down to room temperature (for approximately 20 minutes) before you begin working on it. Do not leave the instrument unattended when the housing is not mounted to the source.

⚠ CAUTION **Hot Surface.** Hot ion source parts might ignite combustible material. During operation of the mass spectrometer, ion transfer capillary and sweep cone might reach temperatures of up to 450 °C. To cool the ion transfer capillary, set the capillary temperature to 25 °C or place the electronics service switch in the Service Mode position. Wait until the ion source has cooled down to room temperature (for approximately 20 minutes) before you begin working on it. Keep combustible materials away from the ion source mount. Do not leave the instrument unattended when the housing is not mounted to the source.

⚠ CAUTION **High Temperatures.** Burn Hazard. When the reagent ion source is in Off mode, restrictor oven, transfer line, and ion source remain at 160 °C.

⚠ CAUTION **High Temperatures.** Burn Hazard. Do not try to handle the vials or vial holders when the cooling nitrogen stops. They are still too hot to handle when the cooling nitrogen stops at a vial temperature of 70 °C. Follow the procedures in “Replacing the Reagent Vials” on page 6-50 if it is necessary to install or replace the reagent vials.

⚠ CAUTION **High Temperatures.** Burn Hazard. If the water circuit fails, all parts of the water distribution unit might be considerably heated up. Do not touch the parts! Before you disconnect the cooling water hoses, make sure that the cooling water has cooled down!

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 white nitrile clean room gloves from Fisher Scientific or Unity Lab Services.

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

EMC Information

In accordance with our commitment to customer service and safety, this instrument has satisfied the requirements for the European CE Mark including the Low Voltage Directive.

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 might result in instrument damage and/or operator injury.

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.

Chapter 4 Installation

This chapter describes the conditions for an operating environment that will ensure continued high performance of your Orbitrap Elite system.

Contents

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

Safety Guidelines for Installation

When you install the Orbitrap Elite 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. Most of the nitrogen that is introduced into the API source (about 5000 L or 180 ft^3 per day) escapes into the laboratory atmosphere. Ensure that the laboratory is well ventilated. Always operate Orbitrap Elite mass spectrometer and API source with attached drain tubing assembly that connects the source housing drain to a dedicated exhaust system.

⚠ WARNING

Hazardous Chemicals. The effluent of the forepumps might contain noxious chemicals. The forepumps eventually exhaust much of what is introduced into the mass spectrometer, including the small amount of oil vapor that mechanical pumps can emit. The connection to an adequate exhaust system is mandatory!

⚠ WARNING

Hazardous Chemicals. The source exhaust might contain noxious material. It will contain traces of the samples and solvents that you are introducing into the source. Potential health hazards of these compounds include chemical toxicity of solvents, samples, and buffers, as well as biohazards of biological samples. To prevent contamination of the laboratory, always operate the ion source with the drain tubing connected. The drain tubing must lead to a waste container that is connected to a dedicated fume exhaust system.

⚠ 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

The Orbitrap Elite instrument has dimensions of *l* 1462.5 mm (58 in.), *w* 870 mm (35 in.), *h* 1414 mm (56 in.). See Figure 4-1.

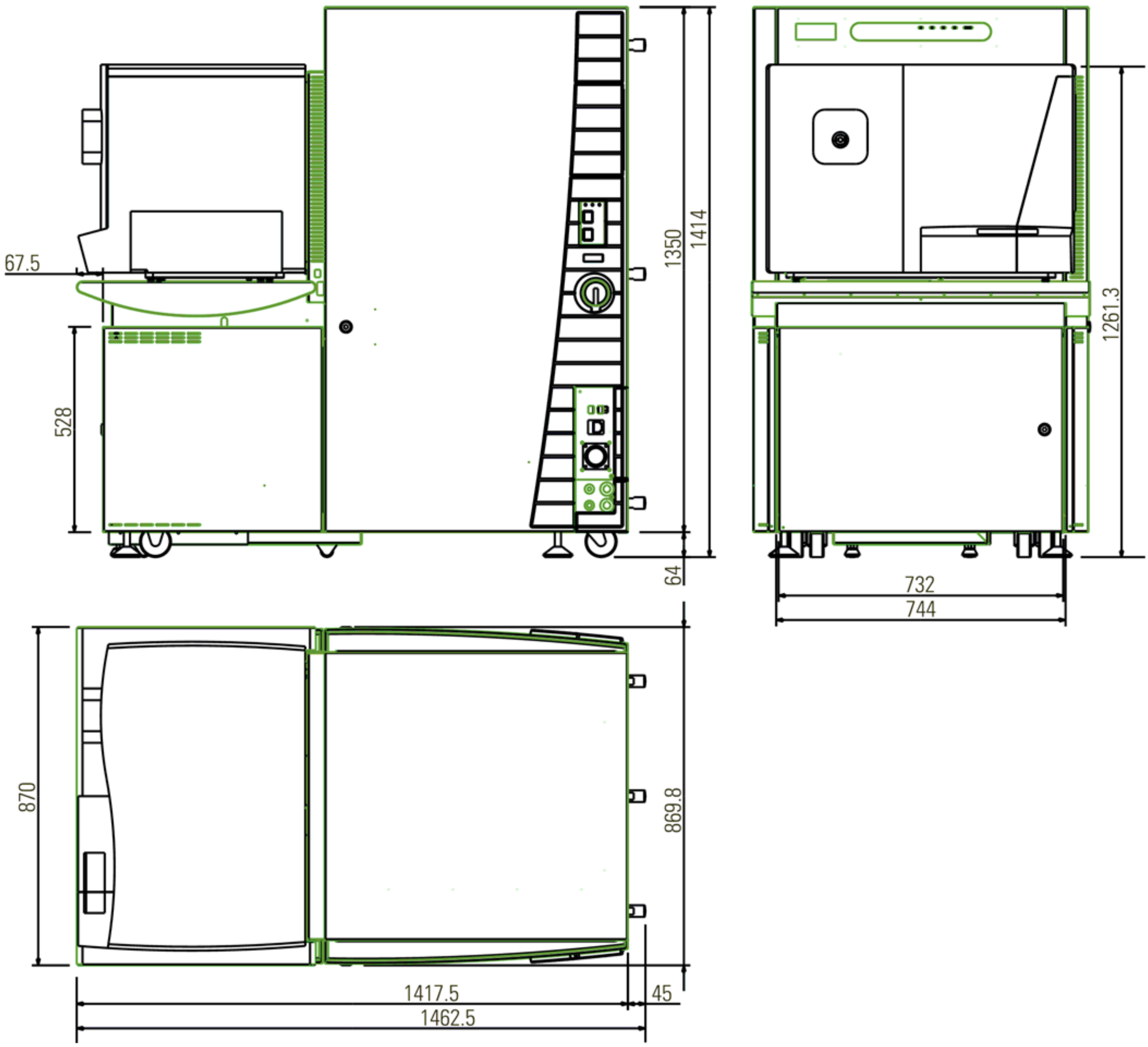


Figure 4-1. Dimensions of Orbitrap Elite MS in mm

In the Orbitrap Elite ETD system, the ETD Module is attached to the rear of the instrument. The instrument has maximum dimensions of *l* 1705 mm (67 in.), *w* 913 mm (36 in.), h 1414 mm (56 in.).

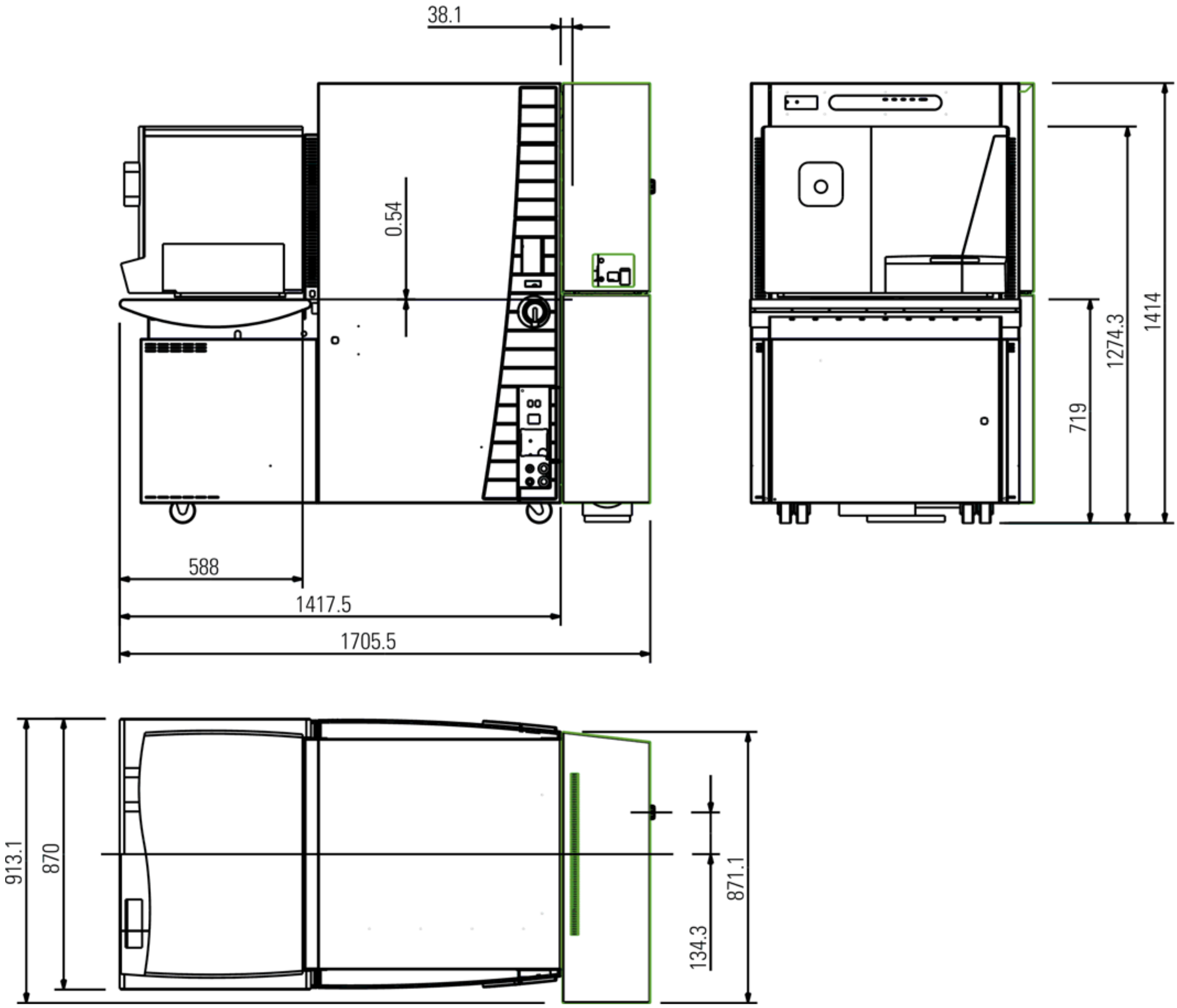


Figure 4-2. Important dimensions of Orbitrap Elite ETD MS

Load Distribution

The Orbitrap Elite instrument is supported by four height adjustable feet. The floor of your laboratory should be able to carry the weight of the installed Orbitrap Elite instrument with data system and recirculating chiller of about 685 kg (1510 lb). Also, consider the weight of any other option that is added to the system.

The components of the ETD system weigh approximately 125 kg (276 lb), including the ETD Module, the transfer mechanics, and the pumps.

Laboratory Conditions

This section gives an overview of important requirements for the laboratory where the Orbitrap Elite mass spectrometer is placed. For details, refer to the *LTQ Orbitrap Series Preinstallation Requirements Guide*.

Power Supply

Table 4-1. Power Supply

System Component	Requirements
Instrument	230 V AC ± 10% 3 phase, 15 Ampere, 50/60 Hz, with earth ground
Data System[a]	120 or 230 V AC single phase, 15/16 Ampere, with earth ground
Recirculation chiller	120 or 230 V AC single phase, 15/16 Ampere, with earth ground

[a] The Orbitrap Elite MS provides electric power for the data system. The Orbitrap Elite ETD MS provides electric power for the ETD Module and the data system is connected to a wall outlet.

Gas Supply

Table 4-2. Gas Supply

Gas	Requirements
Helium	Ultra-high purity (99.999%) with less than 1 ppm each of water, oxygen and total hydrocarbons. The required gas pressure is 275 ± 70 kPa (40 ±10 psi).
Nitrogen	High purity (99.5% pure, flow rate 15 L/min) nitrogen gas supply for the API source, the C-Trap, the HCD collision cell, and for cooling the reagent vials of the Orbitrap Elite ETD MS. The required gas pressure is 690 ± 140 kPa (100 ± 20 psi).
ETD Reagent Carrier Gas	Recommendation: A mixture of 25% helium and 75% nitrogen. This gas mixture must be ultra high-purity (minimum purity 99.999%) with less than 3.0 ppm each of water, oxygen, and total hydrocarbons. The required gas pressure is 690 ± 140 kPa (100 ± 20 psi). If the helium/nitrogen mixture is not available: Ultra-high purity nitrogen (UHP, 99.999%) with less than one ppm each water and oxygen.

❖ **To connect the nitrogen source to the Orbitrap Elite mass spectrometer**

1. Connect an appropriate length of Teflon™ tubing to the nitrogen source in the laboratory. The Installation Kit contains 6 m (20 ft) of suitable Teflon tubing. 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 opposite end of the Teflon tubing to the press-in fitting labeled Nitrogen, which is at the right side of the instrument. See Figure 2-9 on page 2-10. To connect the tubing, align the Teflon tubing with the opening in the fitting and firmly push the tubing into the fitting until the tubing is secure.

❖ **To connect the helium source to the Orbitrap Elite mass spectrometer**

1. Connect an appropriate length of 1/8-in. ID copper or stainless steel tubing with a brass Swagelok™-type 1/8-in. nut and a 2-piece brass 1/8-in. ID ferrule to the Helium gas inlet. See Figure 4-3 for the proper orientation of the fitting and ferrule.

2. Connect the opposite end of the tubing to the helium gas source, using an appropriate fitting.

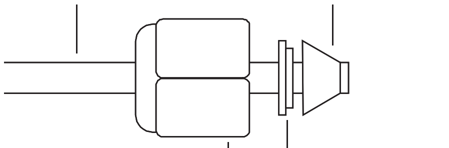


Figure 4-3. Proper orientation of the Swagelok-type nut and two-piece ferrule

Cooling Water

The Orbitrap Elite MS is shipped with a Thermo Scientific ThermoFlex 900 recirculating chiller with closed circuit, cooled by a refrigerating device. The chiller makes the mass spectrometer independent from any cooling water supply.

Use a wall outlet to provide the electric power for the chiller. (See Table 4-1 on page 4-5 for specifications.) Two water hoses (black), internal diameter 9 mm, wall thickness 3 mm, length approximately 3 m (~10 ft) are shipped with the instrument. The hoses are connected to the ports at the right side of the MS.

Table 4-3. Technical Data of Recirculating Chiller

Property	Specification
Cooling capacity	0.90 kW (60 Hz), 0.75 kW (50 Hz)
Water temperature	5–40 °C (41–104 °F)
Stability of temperature regulation	±0.1 °C (±32.2 °F)
Unit dimensions (*h* × *w* × *l*)	69.4 cm × 35.7 cm × 62.4 cm (27 $^{5}/_{16}$ in. × 14 $^{1}/_{16}$ in. x 24 $^{9}/_{16}$ in.)
Unit weight	57.2 kg (126 lb)

Water Conditions

The water temperature is not critical, but should be in the range of 20 to 25 °C (68 to 77 °F). Lower temperatures could lead to a condensation of atmospheric water vapor. It is recommended to use distilled water rather than de-ionized water due to lower concentration of bacteria and residual organic matter.

The water should be free of suspended matter to avoid clogging of the cooling circuit. In special cases, an in-line filter is recommended to guarantee consistent water quality. See Table 4-4 for the cooling water requirements.

Table 4-4. Cooling Water Requirements

Property	Specification
Hardness	<0.05 ppm
Resistivity	1–3 MΩ/cm
Total dissolved solids	<10 ppm
pH	7–8

Environment

The temperature of operating environment must be 16–26 °C (59–78 °F) and the relative humidity must be 50–80% with no condensation. The optimum operating temperature is 18–21 °C (65–70 °F)

The system averages 2800 W (10000 Btu/hr) output when considering air conditioning needs. With ETD, the system averages 3500 W (12000 Btu/hr) output.

Ventilation and Fume Exhaust

Most of the nitrogen that is introduced into the API source (about 5000 L or 180 ft^3 per day) escapes into the laboratory atmosphere. Therefore, provide for good air exchange to prevent accumulation of gaseous nitrogen in the laboratory.

The exhaust port of the rotary pumps should be connected to an exhaust gas line leading out of the building or exhaust system. The inner diameter of the pipe should be at least 25 mm (1 in.). An exhaust hose for connecting the forepumps to the exhaust system comes with the system and is 5 m (16 ft) long. It has dimensions of 13 mm (1/2 in.) ID and 20 mm (25/32 in.) OD. The exhaust system for the forepumps must be able to accommodate an initial inrush flow rate of 3 L/min and a continuous flow rate of 1 L/min.

⚠ Do not vent the drain tubing (or any vent tubing connected to the waste container) to the same fume exhaust system to which you have connected the forepumps.

Chapter 5 Basic System Operations

Many maintenance procedures for the Orbitrap Elite system require that the mass spectrometer be shut down. In addition, the Orbitrap Elite system can be placed in Standby condition if the system is not to be used for 12 hours or more.

Contents

Safety Guidelines for Operation

When you operate the Orbitrap Elite system, pay attention to the following general safety guidelines.

⚠ WARNING

High Voltage. If you touch liquid leaking from the probe sample inlet while the mass spectrometer is in operation, you might receive an electric shock. Do not tighten the probe sample inlet fitting to eliminate a liquid leak while the mass spectrometer is in operation.

⚠ WARNING

Suffocation Hazard. Accumulation of nitrogen gas could displace sufficient oxygen to suffocate personnel in the laboratory. Most of the nitrogen that is introduced into the API source (about 5000 L or 180 ft^3 per day) escapes into the laboratory atmosphere. Ensure that the laboratory is well ventilated. Always operate Orbitrap Elite mass spectrometer and API source with attached drain tubing assembly that connects the source housing drain to a dedicated exhaust system.

⚠ WARNING

Hazardous Chemicals. The effluent of the forepumps might contain noxious chemicals. The forepumps eventually exhaust much of what is introduced into the mass spectrometer, including the small amount of oil vapor that mechanical pumps can emit. The connection to an adequate exhaust system is mandatory!

⚠ WARNING

Hazardous Chemicals. The source exhaust might contain noxious material. It will contain traces of the samples and solvents that you are introducing into the source. Potential health hazards of these compounds include chemical toxicity of solvents, samples, and buffers, as well as biohazards of biological samples. To prevent contamination of the laboratory, always operate the ion source with the drain tubing connected. The drain tubing must lead to a waste container that is connected to a dedicated fume exhaust system.

⚠ 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.** The external surface of the ion source housing can become hot enough to burn your skin. Do not touch the ion source housing when the mass spectrometer is in operation. Let the ion source housing cool to room temperature (approximately 60 minutes) before you touch it or remove it from the mass spectrometer.

CAUTION **Hot Surface.** Hot ion source parts might ignite combustible material. During operation of the mass spectrometer, ion transfer capillary and sweep cone might reach temperatures of up to 450 °C. To cool the ion transfer capillary, set the capillary temperature to 25 °C or place the electronics service switch in the Service Mode position. Wait until the ion source has cooled down to room temperature (for approximately 60 minutes) before you begin working on it. Keep combustible materials away from the ion source mount. Do not leave the instrument unattended when the housing is not mounted to the source.

CAUTION **Hot Surface.** Touching hot parts of the ion source interface might cause severe burns. During operation of the mass spectrometer, ion transfer capillary and sweep cone might reach temperatures of up to 450 °C. Do not touch the ion source mount immediately after removing the ion source housing. To cool the ion transfer capillary, set the capillary temperature to 25 °C or place the electronics service switch in the Service Mode position. 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 housing is not mounted to the source.

Placing the Instrument in Standby Condition

The Orbitrap Elite 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. When you are not going to operate the system for 12 hours or more, you can leave the system in Standby condition.

In case of an Orbitrap Elite ETD mass spectrometer, first place the ETD Module in Standby condition. Then place the mass spectrometer in Standby condition according to the procedures described in the following topics.

Placing the ETD Module in Standby Condition

❖ **To place the ETD Module in Standby condition**

1. If the Tune Plus window is not already open, choose **Start > Programs > Thermo Instruments > LTQ > LTQ Tune** from the taskbar. The Tune Plus window will open.

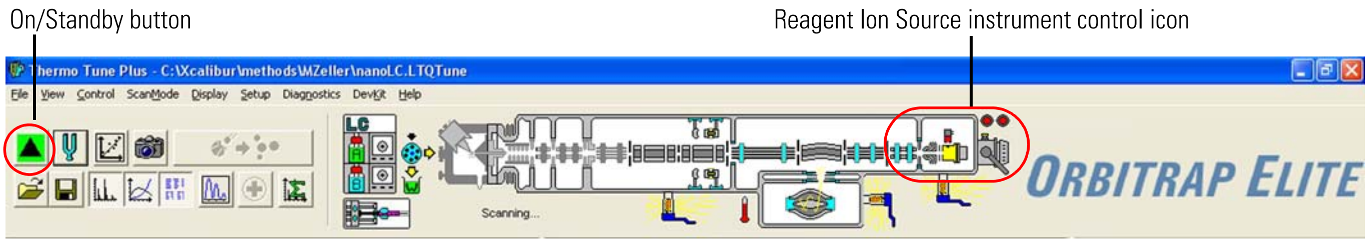
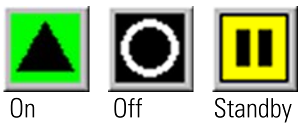


Figure 5-1. Tune Plus window (Orbitrap Elite ETD), toolbar



You can determine the state of the mass spectrometer by observing the state of the On/Off/Standby button on the Control/Scan Mode toolbar. See Figure 5-1. The three different states of the On/Standby button are shown at the left.

2. Click the Reagent Ion Source portion of the instrument control graphic at the top of the Tune Plus window. (See Figure 5-1.) The Reagent Ion Source dialog box appears. (See Figure 5-2.)

3. In the Reagent Ion Source dialog box, clear the Reagent Ion Source On box to place the Reagent Ion Source in Standby condition. See Figure 5-2 on page 5-5. This places the Reagent Ion Source in Standby condition as indicated by the Actual condition shown to the right of the Reagent Ion Source On box.

   When the reagent ion source is placed in Standby condition, the filament and vial heaters turn off. Simultaneously, a valve opens to allow the nitrogen gas to cool the reagent vials. This cooling nitrogen runs until the reagent vials reach 70 °C. The audible rush (hissing noise) of nitrogen from the reagent ion source area in the back of the ETD Module is normal operation.

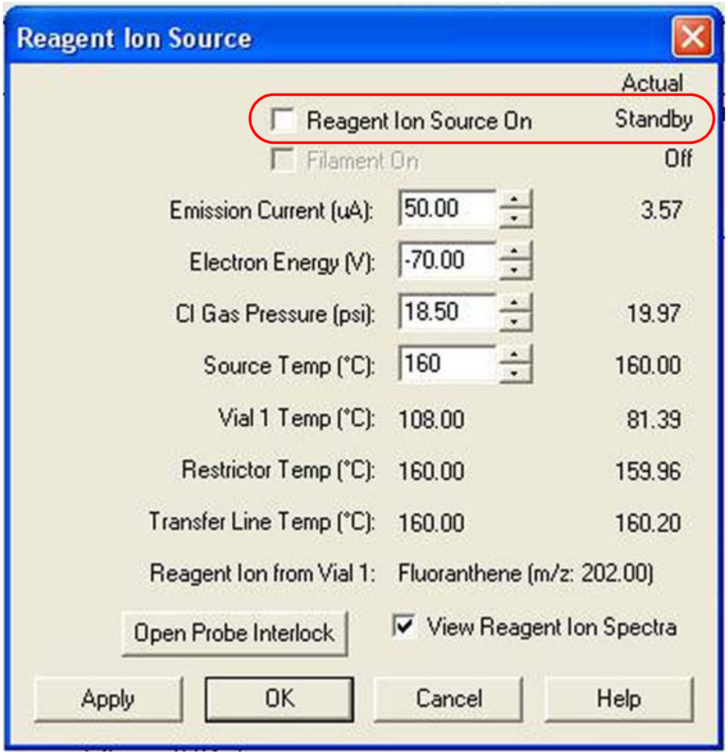


Figure 5-2. Reagent Ion Source dialog box with Reagent Ion Source On box and Actual condition circled

If the reagent ion source is on when you place the Orbitrap Elite ETD mass spectrometer in Standby mode, the filament turns off immediately. In contrast, the vial heaters stay on for 60 minutes before they turn off and the cooling gas begins. Because the filament is turned off, you can perform minor maintenance procedures on the ETD Module without cooling the reagent inlet.

⚠ CAUTION

High Temperatures. Burn Hazard. The reagent vials will be too hot to touch after the cooling nitrogen turns off at 70°C. Install or exchange the reagent vials by following the procedure in "Replacing the Reagent Vials" on page 6-50. Make sure that the reagent vials are cool to the touch before handling them.

More information about turning on and off the reagent heaters is given in "Reagent Heaters" on page 2-27.

⚠ CAUTION **High Temperatures.** Burn Hazard. The restrictor, the transfer line, and the ion source heater operate at 160 °C. Do not touch them unless the Orbitrap Elite mass spectrometer is shut down (See “Shutting Down the Orbitrap Elite Mass Spectrometer Completely” on page 5-7.) and these heaters have had sufficient time to cool down to room temperature.

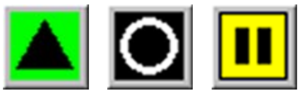
Placing the MS in Standby Condition

❖ **To place the Orbitrap Elite system in Standby condition**

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

2. Turn off the flow of solvent from the LC (or other sample introduction device).

   NOTICE For instructions on how to operate the LC from the front panel, refer to the manual that came with the LC. ▲



3. From the Tune Plus window, choose **Control > Standby** (or click on the **On/Standby** button to toggle it to Standby) to put the instrument in Standby condition. The consequences of this user action are described in the *LTQ Series Hardware Manual*. The System LED on the front panel of the Velos Pro mass spectrometer turns yellow when the system is in Standby condition.

4. Leave the LC power on.

5. Leave the autosampler power on.

6. Leave the data system power on.

7. Leave the Orbitrap Elite MS main power switch in the On position.

Shutting Down the Orbitrap Elite Mass Spectrometer Completely

The Orbitrap Elite mass spectrometer 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 weekends. Shut down ETD Module and MS system completely only if you do not want to use them for an extended period or if you want to perform a maintenance or service procedure.

❖ **To shut down the instrument completely**

1. Place the ETD Module in Standby condition as described in "Placing the ETD Module in Standby Condition" on page 5-4.

2. Shut down the instrument as described in "Shutting Down the Instrument" below. This also shuts down the ETD Module because its power controls are linked to the Orbitrap Elite MS power controls through the ETD Module Interface board. See "ETD Module Interface Board" on page 2-25.

Shutting Down the Instrument

❖ **To shut down the Orbitrap Elite system**

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

2. Turn off the flow of solvent from the LC (or other sample introduction device).

   NOTICE For instructions on how to operate the LC from the front panel, refer to the manual that came with the LC. ▲

3. From the Tune Plus window, choose **Control > Off** to put the instrument in Off condition. When you choose **Control > Off**, all high voltages are shut off, as are the flows of the sheath gas and the auxiliary gas.

4. Put the FT Electronics switch to the Off position. See Figure 2-7 on page 2-8.

5. Put the Vacuum Pumps switch to the Off position. See Figure 2-7. When you place the switch in the Off position, the following occurs:

   a. All power to the instrument, including the turbomolecular pumps and the rotary-vane pumps, is turned off.

   b. After 30 seconds, power to the vent valve solenoid of the ion trap is shut off. The vent valve opens and the vacuum manifold is vented with nitrogen to atmospheric pressure through a filter. You can hear a hissing sound as the gas passes through the filter.

6. Leave the main power switch of the Orbitrap Elite mass spectrometer in the On position.

7. During service or maintenance operations that require opening the vacuum system of the Velos Pro MS or the Orbitrap Elite MS, always put the main switch (main circuit breaker) to the Off position. You can secure the main switch with a padlock or tie-wrap to prevent unintended re-powering.

⚠ CAUTION **High Temperatures.** Burn Hazard. Let heated components cool down before you service them (the ion transfer tube is operated at about 300 °C, for example).

NOTICE If you are planning to perform routine or preventive system maintenance on the Orbitrap Elite mass spectrometer only, you do not need to switch off the recirculating chiller, LC, 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 recirculating chiller, LC, autosampler, and data system. ▲

Starting up the System after a Shutdown

To start up the Orbitrap Elite mass spectrometer after it has been shut down, you need to do the following:

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

Starting up the Instrument

NOTICE The recirculating chiller and data system must be running before you start up the instrument. The instrument will not operate until it has established a communication link to the data system. ▲

❖ **To start up the Orbitrap Elite mass spectrometer**

1. Start up the (optional) LC and autosampler as is described in the manual that came with the LC and autosampler.
2. Start up the data system and the chiller.
3. Turn on the flows of helium and nitrogen at the tanks, if they are off.
4. Make sure that the main power switch of the Velos Pro MS is in the On position and the electronics service switch of the Velos Pro MS is in the Operating position.
5. Place the main power switch at the right side of the Orbitrap Elite mass spectrometer in the On position.
6. Put the Vacuum Pumps switch to the On position. See Figure 2-7 on page 2-8. The rotary-vane pumps and the turbomolecular pumps are started.

   NOTICE Pumping the system after a complete shut down takes hours and requires overnight baking of the system. ▲

7. Put the FT Electronics switch to the On position. See Figure 2-7. When you place the FT Electronics switch to the On position, the following occurs:

   a. Power is provided to all electronic boards. (The electron multiplier, conversion dynode, 8 kV power to the API source, main RF voltage, and quadrupole RF voltage remain off.)

   b. The internal computer reboots. After several seconds, the Communication 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 Communication 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 three minutes, the System LED of the ion trap turns yellow to indicate that the software transfer from the data system is complete and that the instrument is in Standby condition.

NOTICE The Vacuum LED on the front panel of the Velos Pro turns green only if the pressure in the vacuum manifold is below the maximum allowable pressure (5×10^{-4} Torr in the analyzer region, and 2 Torr in the S-lens region), and the safety interlock switch on the API source is pressed down (that is, the API flange is secured to the spray shield). ▲

8. Press the Reset button on the Velos Pro mass spectrometer to establish the communication link between Velos Pro MS and internal computer.

If you have an LC or autosampler, start it as is described in the manual that came with the LC or autosampler. Then, proceed to "Setting up Conditions for Operation". If you do not have either, go to the topic directly.

Setting up Conditions for Operation

❖ **To set up your Orbitrap Elite mass spectrometer for operation**

1. Before you begin data acquisition with your Orbitrap Elite system, you need to allow the system to pump down for at least eight hours. Operation of the system with excessive air and water in the vacuum manifold can cause reduced sensitivity, tuning problems, and a reduced lifetime of the electron multiplier.

   NOTICE The vacuum in the analyzer system can be improved by an overnight baking of the system. See "Baking Out the System" on page 6-6. ▲

2. Ensure that the gas pressures are within the operational limits:

   - Helium: 275 ± 70 kPa (2.75 ± 0.7 bar, 40 ±10 psi),
   - Nitrogen: 690 ± 140 kPa (6.9 ± 1.4 bar, 100 ± 20 psi).

In case of an Orbitrap Elite ETD mass spectrometer, also check the pressure of the reagent carrier gas: 690 ± 140 kPa (6.9 ± 1.4 bar, 100 ± 20 psi).

NOTICE Air in the helium line must be purged or given sufficient time to be purged for normal performance. ▲

3. Click the **Display Status View** button in the Tune Plus window. Check whether the pressure measured by the ion gauge is $\leq 5 \times 10^{-9}$ mbar, and the pressure measured by the Pirani gauge is around 1 mbar. Compare the values of the other parameters in the status panel with values that you recorded previously.

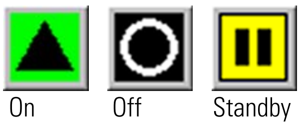
4. In case of an Orbitrap Elite ETD mass spectrometer, start up the ETD Module as described in "Starting the ETD Module after a Complete Shutdown". In case of an Orbitrap Elite MS, continue to set up for ESI or APCI operation as described in *Orbitrap Elite Getting Started*.

Starting the ETD Module after a Complete Shutdown

❖ **To start up the ETD Module after a complete shutdown**

1. Start the Orbitrap Elite ETD mass spectrometer according to the start up procedures given in "Starting up the System after a Shutdown" above. This also turns on the ETD Module as the ETD Module power controls are linked to the MS power controls (see "ETD Module Interface Board" on page 2-25).

2. If the Tune Plus window is not already open, choose **Start > Programs > Thermo Instruments > LTQ > LTQ Tune** from the task bar. The Tune plus window will open.



You can determine the state of the MS detector by observing the state of the On/Off/Standby button on the Control/Scan Mode toolbar. (See Figure 5-1 on page 5-4.) The three different states of the On/Standby button are shown at the left.

3. Click the **Display Status View** button in the Tune Plus window.

   Check the reagent vacuum parameters:

   - Reagent ion gauge pressure: 20 to 35 × 10^{-5} Torr
   - Reagent Convectron gauge pressure: <0.08 Torr
   - Reagent turbomolecular pump speed: > 90%

4. Continue to set up the instrument for operation as described in *Orbitrap Elite Getting Started* manual.

Resetting the System

If the communication link between Orbitrap Elite mass spectrometer and data system computer is lost, it may be necessary to reset the system using the Reset button of the Velos Pro mass spectrometer.

The procedure given here assumes that the Orbitrap Elite mass spectrometer and data system computer are both powered on and are operational. If the instrument, data system computer, or both are off, see "Starting up the System after a Shutdown" on page 5-9.

To reset the Orbitrap Elite mass spectrometer, press the Reset button of the Velos Pro. See the *LTQ Series Hardware Manual* for the location of the Reset button. When you press the Reset button, the following occurs:

1. An interrupt on the mainboard of the internal computer causes the internal computer to reboot. All LEDs on the front panel are off except the Power LED.
2. After several seconds, the Communication LED turns yellow to indicate that the data system and the instrument are starting to establish a communication link.
3. After several more seconds, the Communication 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.
4. After three 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.

Resetting Tune and Calibration Parameters to their Default Values

You can reset the Orbitrap Elite system tune and calibration parameters to their default values at any time. This feature may be useful if you have manually set some parameters that have resulted in less than optimum performance.

❖ **To reset the Orbitrap Elite MS tune and calibration parameters**

In the Tune Plus window,

- Choose **File > Restore Factory Calibration** to restore the default calibration parameters, or
- Choose **File > Restore Factory Tune Method** to restore the default tune parameters.

NOTICE Make sure that any problems you might be experiencing are not due to improper API source settings (spray voltage, sheath and auxiliary gas flow, ion transfer capillary temperature, etc.) before resetting the system parameters to their default values. ▲

Turning off the Reagent Ion Source: What to Expect

In the Orbitrap Elite ETD mass spectrometer, the reagent ion source controls can be accessed as described in “Placing the ETD Module in Standby Condition” on page 5-4. When you clear the Reagent Ion Source On check box in the Reagent Ion Source dialog box (See Figure 5-3.), the ETD source and reagent heaters are placed in Standby condition.

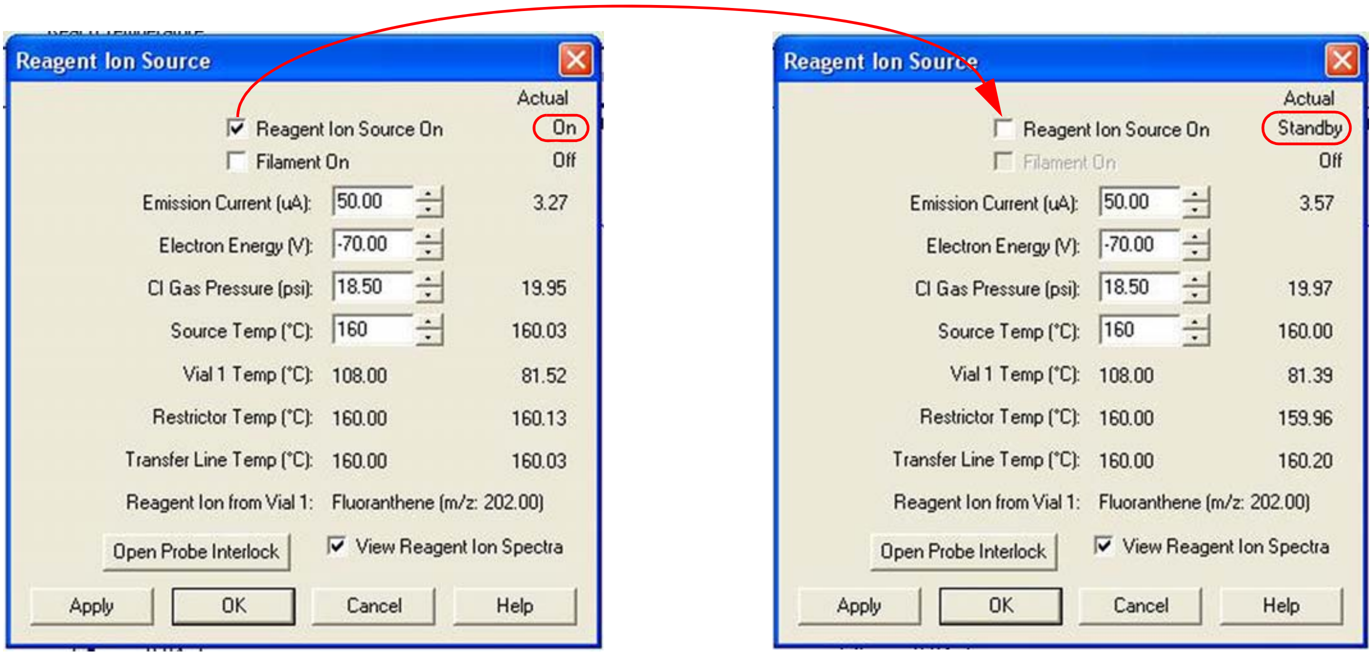


Figure 5-3. Placing the reagent ion source in Standby condition

When the ETD Module is placed in Standby condition, the filament and vial heaters are turned off. Simultaneously a valve opens to allow nitrogen gas to cool the reagent vials. This cooling nitrogen runs until the vials reach 70 °C. The audible rush (hissing noise) of nitrogen from the reagent ion source area in the back of the ETD Module is normal operation.

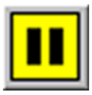
⚠ CAUTION

High Temperatures. Burn Hazard. The reagent vials are too hot to handle after the cooling nitrogen turns off at a vial temperature of 70 °C. Make sure that the reagent vials have cooled down to a safe temperature before handling them. This can take up to 90 minutes after the cooling nitrogen has turned off.

Other conditions that will cause the ETD Module to remain in Standby:

- Trying to turn on the reagent ion source when the restrictor heater, transfer line heater, and the source heater are not at their target temperatures.

- When either the mass spectrometer or the ETD Module goes into Standby mode. Reagent vial nitrogen cooling will turn on if the vials are at an elevated temperature.



Exception: If the Orbitrap Elite ETD mass spectrometer is placed in Standby by clicking the Standby button in Tune Plus (see Standby icon in the margin), there is an hour delay before the cooling nitrogen turns on. ▲

- When the pressure in the mass spectrometer or the ETD Module exceeds its protection limit. Reagent vial nitrogen cooling will turn on if the vials are at an elevated temperature.

- When the abundance of reagent ions becomes insufficient as determined by the AGC setting. When this occurs, the Orbitrap Elite ETD mass spectrometer completes the Xcalibur Sequence step in progress before going into Standby mode.

Chapter 6 User Maintenance

This chapter describes routine maintenance procedures that must be performed to ensure optimum performance of the Orbitrap Elite mass spectrometer.

For instructions on maintaining the Velos Pro linear trap, refer to the *LTQ Series Hardware Manual*. For instructions on maintaining LCs or autosamplers, refer to the manual that comes with the LC or autosampler.

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

Contents

Safety Guidelines for Maintenance

When you perform maintenance on the Orbitrap Elite 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 the mass spectrometer before you try any type of maintenance.

⚠ CAUTION

Hot Surface. Touching parts of the forepumps might cause burns. Forepump in function is hot and some surfaces could reach a temperature higher than 80 °C (176 °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. Hot ion source parts might ignite combustible material. During operation of the mass spectrometer, ion transfer capillary and sweep cone might reach temperatures of up to 450 °C. To cool the ion transfer capillary, set the capillary temperature to 25 °C or place the electronics service switch in the Service Mode position. Wait until the ion source has cooled down to room temperature (for approximately 20 minutes) before you begin working on it. Keep combustible materials away from the ion source mount. Do not leave the instrument unattended when the housing is not mounted to the source.

⚠ CAUTION

Hot Surface. Touching hot parts of the ion source interface might cause severe burns. During operation of the mass spectrometer, ion transfer capillary and sweep cone might reach temperatures of up to 450 °C. Do not touch the ion source mount immediately after removing the ion source housing. To cool the ion transfer capillary, set the capillary temperature to 25 °C or place the electronics service switch in the Service Mode position. Wait until the ion source has cooled down to room temperature (for approximately 20 minutes) before you begin working on it. Do not leave the instrument unattended when the housing is not mounted to the source.

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.

Do not 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 Remarks

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 6-1.

Table 6-1. User maintenance procedures

MS Component	Procedure	Frequency	Procedure Location
Analyzer	System bakeout	If necessary (for example, after performing maintenance work on the vacuum system)	page 6-6
Rotary-vane pumps	Add oil	If oil level is low	Manufacturer's documentation
	Change oil	Every three months or if oil is cloudy or discolored	Manufacturer's documentation page 6-7
Turbomolecular pumps	Replace operating fluid reservoir and pump bearings	Every four years	Manufacturer's documentation page 6-14
Cooling water circuit	Check cooling fluid level Check cooling fluid filter Check air inlet filter	See manufacturer's documentation	Manufacturer's documentation page 6-60
	Replace filter cartridge	Annually	page 6-60
ETD Module	Clean ion volume	As needed[a]	page 6-24
	Replace inlet valve components	As needed[a]	page 6-47
	Clean ion source lenses	As needed[a]	page 6-36
	Clean ion source	As needed[a]	page 6-42
	Replace ion source filament	As needed[a]	page 6-44
	Replace reagent vials	As needed[a]	page 6-50
	Check rotary-vane pump oil and add when needed	Every month	page 6-10
	Change rotary-vane pump oil	Every four months	page 6-12
	Clean rear cooling fans	Every four months	page 6-59

[a] As needed depends on how close the component is to the electron transfer reagent introduction point. For example, the ion volume is closer to the fluoranthene introduction point than any other component and requires the most frequent cleaning.

To successfully carry out the procedures listed in this chapter, observe the following rules:

- Proceed methodically.
- Always wear clean, lint-free, and powder-free gloves when handling the components of the API source, ion optics, mass analyzer, and ion detection system. See “Personal Protective Equipment” on page 3-11 for a specification for the required gloves.
- Do not re-use gloves after you remove them because the surface contaminants on them will re-contaminate clean parts.
- Always wear protective eye wear when you clean parts.
- Always place the components on a clean, lint-free, and powder-free surface.
- Always cover the opening in the top of the vacuum manifold with a large, lint-free tissue when you remove the top cover plate of the vacuum manifold.
- Do not 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 Orbitrap Elite mass spectrometer.
- Do not insert a test probe (for example, an oscilloscope probe) into the sockets of female cable connectors on PCBs.

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. ▲

Maintenance of the Vacuum System

This section contains instructions for performing a system bakeout and for performing pumps maintenance.

Baking Out the System

Collected or remaining gases and molecules as well as moisture can lead to an increased number of collisions with sample ions in the high vacuum region of the instrument. The bakeout procedure removes these contaminations. Therefore, we recommend to bake out the instrument if the high vacuum decreases noticeably during routine operation.

Bakeout is mandatory after maintenance or service work is performed in the analyzer region where the system is vented.

NOTICE Pumping down the system after venting takes at least eight hours, and usually requires overnight baking of the system. ▲

If the system has been vented during a power failure, then it is necessary to bake out the system to obtain the operating vacuum. See "Behavior of the System in Case of a Main Failure" on page 3-8.

Bakeout Procedure

❖ **To perform a system bakeout**

1. Put the system in Standby condition as described in "Placing the Instrument in Standby Condition" on page 5-4.

2. Put the FT Electronics switch at the power control panel into the On position.

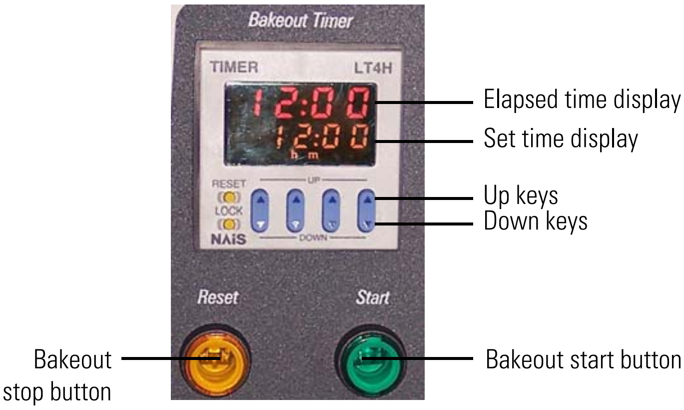


Figure 6-1. Bakeout timer

3. To set the bakeout time, enter the time (hh:mm) with the up/down keys of the bakeout timer. See Figure 6-1.

4. To start the bakeout procedure, press the green start button on the right. The Orbitrap Elite mass spectrometer indicates a running bakeout procedure by the flashing Vacuum LED and System LED at the front side of the instrument. See Figure 2-4 on page 2-5.

   To stop a running bakeout procedure, press the orange reset/stop button on the left side. Also press this button after you have changed the preset bakeout time.

5. The bakeout procedure is terminated because of two reasons:

   - The preset duration has expired, or

   - The vacuum has risen above a preset value.

The termination of the baking process is indicated by the status LEDs (System and Vacuum) on the front side that have stopped flashing.

Maintenance of the Forepumps

Rotary-vane pumps require minimal maintenance. All that is required to maintain the rotary-vane pump is to inspect, add, purge, and change the pump oil.

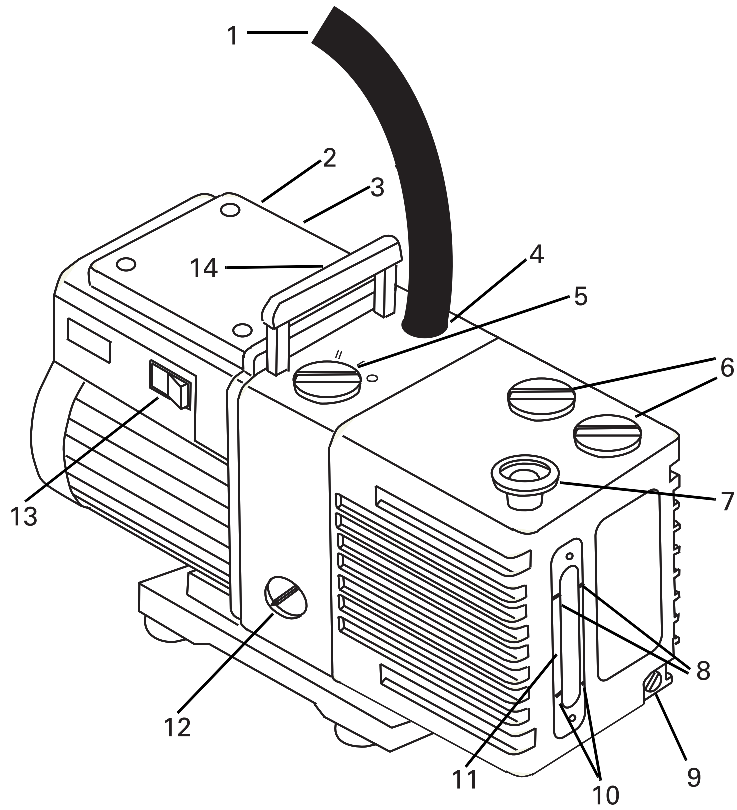
For maintenance of the forepumps of the MS portion, refer to the *LTQ Series Hardware Manual* or the pump manufacturer's manual.

NOTICE The manuals of the pump manufacturers give detailed advice regarding safety, operation, maintenance, and installation. Please note the warnings and precautions contained in these manuals! ▲

Maintenance of the ETD Forepump

Rotary-vane pump oil is a translucent light amber color and it should be checked often. During normal operation, oil must always be visible in the oil level sight glass between the MIN and MAX marks. If the oil level is below the MIN mark, add oil. If the oil is cloudy or discolored, purge the oil to decontaminate dissolved solvents. If the pump oil is still discolored, change it. You should change the pump oil every 3000 hours (about four months) of operation.

The rotary-vane pump major components are shown in Figure 6-2.



Labeled components: 1=Foreline Vacuum Hose, 2=Electrical Inlet Connector, 3=Voltage Indicator, 4=Inlet Port, 5=Gas Ballast Control, 6=Oil Filler Plugs, 7=Outlet Port, 8=MAX Marks, 9=Oil Drain Plug, 10=MIN Marks, 11=Oil Level Sight Glass, 12=Mode Selector, 13= On/Off Switch, 14=Lifting Handle

Figure 6-2. Schematic of ETD forepump

NOTICE During normal operation, the mode selector switch is set to high-vacuum mode (turned fully clockwise) and the gas-ballast control is closed (0). ▲

Accessing the ETD Forepump

As described in "Forepump of the ETD Module" on page 2-34, the ETD forepump is located in a cabinet at the bottom of the ETD Module. To access the ETD forepump, you have to remove the lower panel as indicated in Figure 6-3.

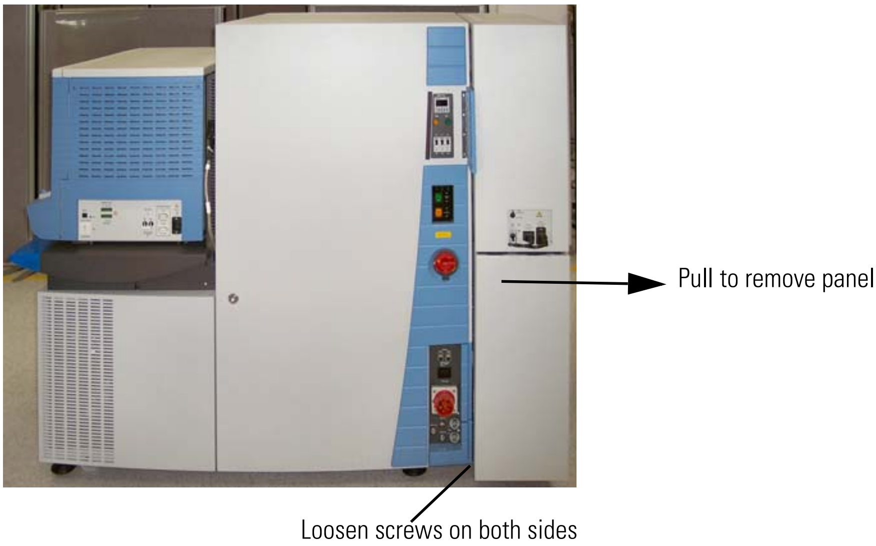


Figure 6-3. Accessing the ETD Forepump: Removing the panel

Two pairs of hooks under the top panel hold the bottom panel. They mount into corresponding openings at the top side of the bottom panel. Figure 6-4 shows the details for the right side of the instrument. The panel hangs on the hooks and comes off if lifted up a little and getting pulled on into the backwards direction.

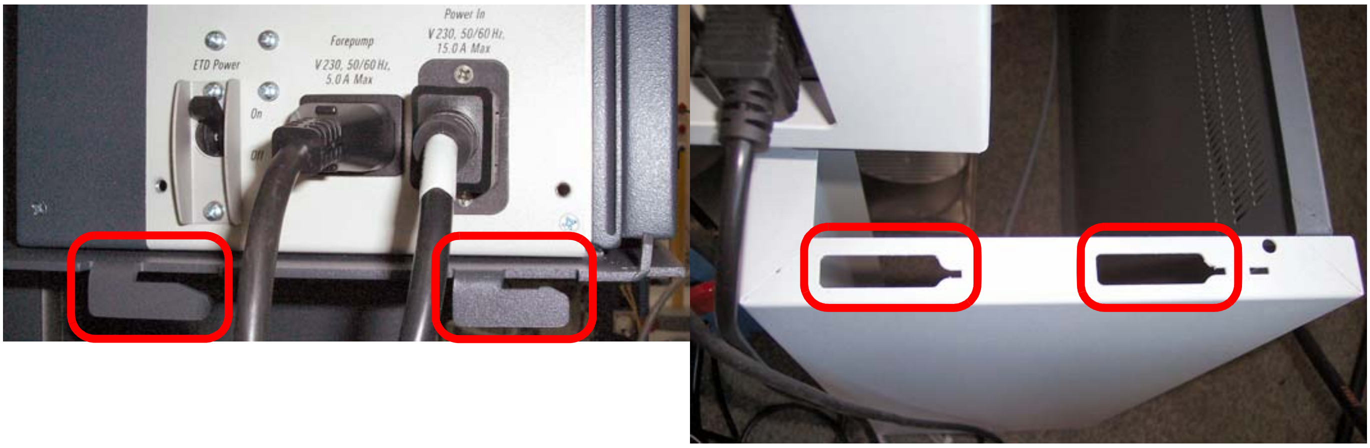


Figure 6-4. Hooks (left) and top side of detached bottom panel (right)

On the bottom of the rear side of the MS portion, two hex screws fix the panel to the instrument frame by means of fork-like extensions (lugs). See Figure 6-5.

Figure 6-5. Lugs for fixing the bottom panel

❖ **To remove the panel**

1. Use a 6 mm hex wrench to loosen the screws that fix the bottom panel. Take care not to loosen the screws completely.

2. Pull the panel horizontally away from the instrument until it comes clear from the hooks.

3. Remove the panel from the instrument and store it at a safe place.

To reattach the panel, proceed in the reverse order.

Adding Oil to the ETD Forepump

The pump oil level must be between the MIN and MAX marks on the oil level sight glass for the pump to operate properly. Pump oil is added as needed when the oil level is below the MIN mark on the oil level sight glass.

You can check the oil level by looking at the oil level sight glass, which is shown in Figure 6-2 on page 6-8. If the ETD forepump oil level is low, follow these steps to add more oil.

❖ **To add oil to the ETD forepump**

1. Shut down and vent the Orbitrap Elite ETD mass spectrometer.

   NOTICE Shut down and unplug the instrument before adding oil. ▲

2. Remove the lower panel at the rear side of the ETD Module as described on page 6-10.

3. Remove one of the oil filler plugs from the rotary-vane pump.

   NOTICE To maintain optimal performance and prevent damage to the ETD forepump, only use factory-approved rotary-vane pump oil. ▲

4. Add fresh oil to the reservoir until the oil is half way between the MIN and MAX level marks. If the oil level goes above the MAX level mark, remove the drain plug and drain the excess oil into a suitable container.

5. Insert the oil filler plug back into the rotary-vane pump.

6. Reattach the lower panel at the rear side of the ETD Module.

7. Plug in the instrument.

8. Restart the system.

Purging the Rotary-Vane Pump Oil

When the rotary-vane pump oil becomes cloudy or discolored, purge the oil. Purging (or decontaminating) the oil removes dissolved gases and low boiling-point liquids. You can purge the oil without interrupting system operation, but do not purge it during an acquisition or while the electron multiplier or filament is powered on.

❖ **To purge the rotary-vane pump oil**

1. Remove the lower panel at the rear side of the ETD Module as described on page 6-10.

2. Set the gas ballast control (See Figure 6-2 on page 6-8.) to Low Flow (I).

3. Operate the pump for 10 minutes or until the oil is clear. If the oil remains cloudy or discolored after 10 minutes, replace the oil.

4. Set the gas ballast control to Closed (0), as shown in Figure 6-6.

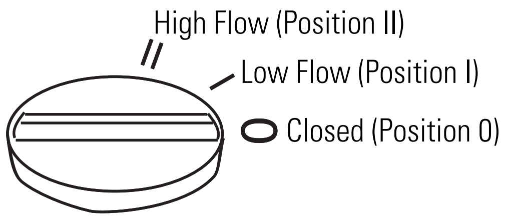


Figure 6-6. Gas ballast control positions

5. Reattach the lower panel at the rear side of the ETD Module.

Changing the Rotary-Vane Pump Oil

You should change the ETD forepump oil every four months (about 3000 hours of operation).

Supplies needed for changing the ETD forepump oil:

- Rotary-vane pump oil
- Suitable container for removing spent or excess oil

NOTICE For best results, change the oil while the ETD forepump is still warm after operation. ▲

⚠ CAUTION **Hot Surface.** Touching parts of the forepump might cause burns. Forepump in function is hot and some surfaces could reach a temperature higher than 80 °C (176 °F). Switch off the pump and let it cool down before any intervention or take appropriate precautions. Always wear heat protective gloves when you work on a pump that is “still warm from operation.”

⚠ CAUTION **High Temperatures.** Burn Hazard. Handle hot pump oil carefully to avoid being burned or injured.

❖ **To change the ETD forepump oil**

1. Shut down and vent the Orbitrap Elite ETD mass spectrometer.

   NOTICE Shut down and unplug the instrument before adding oil. ▲

2. Remove the lower panel at the rear side of the ETD Module as described on page 6-10.

3. Disassemble the rotary-vane pump:

   a. Disconnect the foreline vacuum hose. (See Figure 6-2 on page 6-8.)

   b. Disconnect the exhaust vacuum hose.

   c. Place the rotary-vane pump on a bench.

⚠ CAUTION **Heavy Load.** The ETD forepump weighs 23 kg (50 lb). Use the proper technique when you lift it to prevent muscle strain and back injury.

4. Drain the spent oil:

   a. Remove one of the oil filler plugs.

   b. Remove the oil drain plug and let the oil drain into a suitable container.

   c. Dispose of the spent oil according to local environmental regulations.

   d. Replace the oil drain plug.

5. Add fresh oil:

   a. Add oil into oil filler reservoir half way between the MIN and MAX level marks.

   b. If the oil level goes above the MAX level mark, remove the drain plug and drain the excess oil from the pump.

6. Reassemble the rotary-vane pump:

   a. Replace the oil filler plug.

   b. Return the rotary-vane pump to the floor.

   c. Reconnect the foreline vacuum hose to the rotary-vane pump.

   d. Reconnect the exhaust vacuum hose to the rotary-vane pump.

   e. Plug in the rotary-vane pump.

7. Reattach the lower panel at the rear side of the ETD Module.

8. Plug in the instrument.

9. Restart the system.

Maintenance of the Turbomolecular Pumps

The turbomolecular pumps in the MS portion of the Orbitrap Elite mass spectrometer need maintenance work by the user that is briefly outlined below. In contrast, the turbomolecular pump in the ETD Module of the Orbitrap Elite ETD mass spectrometer contains no user-serviceable parts.

NOTICE The manuals of the pump manufacturers give detailed advice regarding safety, operation, maintenance, and installation. Please note the warnings and cautions contained in these manuals! ▲

Replacing the Operating Fluid Reservoir of the Turbomolecular Pumps

The manufacturer recommends replacing the operating fluid reservoirs of the turbomolecular pumps at least every four years. The storage stability of the operating fluid is limited. The specification of durability is given by the pump manufacturer. The disposal of used oil is subject to the relevant regulations.

Replacements for the operating fluid reservoirs including Porex rods are available from Thermo Fisher Scientific.

NOTICE The pump bearings have also to be replaced at least every four years. This maintenance operation requires special training and additional equipment. Therefore, Thermo Fisher Scientific recommends that you call a Thermo Fisher Scientific field service engineer to replace both the operating fluid reservoir and the pump bearings. ▲

Maintenance of the ETD Module

This section describes routine ETD Module maintenance procedures that must be carried out to ensure optimum performance of the system. Some of the procedures describe how to clean components of the ETD Module. Others involve replacing components or replenishing the electron transfer reagent. See also the *ETD Module Hardware Manual* for additional information.

Figure 6-7 illustrates the sequence in which to perform routine maintenance on the ETD system.

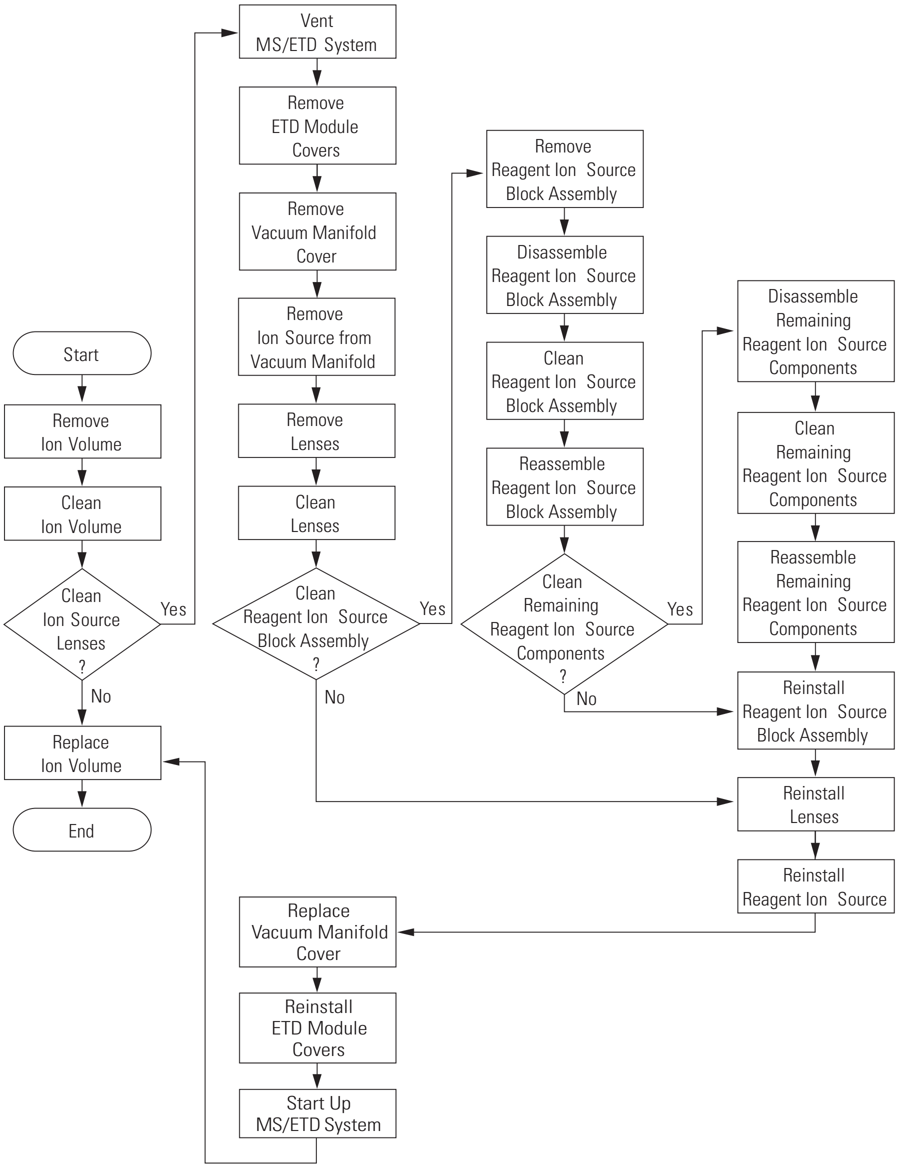


Figure 6-7. Routine maintenance sequence for ETD system

Table 6-2 on page 6-16 gives advice for correcting frequent problems with the ETD system.

Table 6-2. Indications requiring maintenance of the ETD system

Symptom	Cause	Fix
No ions at *m/z* 202 with the emission current at the correct level.	The *m/z* 202 is outside the mass range.	Set the starting mass lower.
The *m/z* 202 signal intensity drops slowly over several days when the emission current is at the correct level.	The ion volume needs to be cleaned or replaced.	Clean or replace the ion volume when the injection time is over 100 ms. See page 6-24.
A system error message advising that the maximum injection time has been reached for the ETD AGC.	The AGC target has not been reached within the specified time limit. The ion volume needs to be cleaned or replaced.	Clean the ion volume. Increase the maximum injection time limit.
Sudden and complete drop of *m/z* 202 level, low emission current.	The filament might just have blown out.	Check the filament. Replace it if necessary. See page 6-44.

Handling and Cleaning Reagent Ion Source Parts

A large part of maintaining your reagent ion source consists of making sure that all the components are clean. Use the cleaning procedures listed in this section to clean stainless steel and non-stainless steel parts. However, use caution when you do so, because some components can be damaged by exposure to liquids.

How often you clean the reagent ion source depends on the amount of reagent introduced into the system. In general, the closer a component is to where the reagent ion is introduced, the more rapidly it becomes dirty (see the footnote in Table 6-1 on page 6-4). For example, the ion volume needs to be cleaned more often than other parts.

Many parts can be removed and disassembled by hand. Make sure that you have all the necessary tools before you carry out a procedure. See below for a list of the tools and supplies that are generally needed for maintenance of the reagent ion source. Tools should be used only for the maintenance of the reagent ion source and be free of grease or other residues. Handle parts in a manner that maintains their cleanliness.

NOTICE It is crucial that the cleanliness of the parts be maintained when they are handled. Wear gloves and place the parts on surfaces that are clean if the parts are not returned directly to the instrument. If clean surfaces are not available, then place the parts on fresh lint free wipes or cloths or aluminum foil that has not been used for any other purpose. ▲

The following tools and supplies are needed for reagent ion source maintenance:

- Clean, dry gas (air or nitrogen)
- New, white nitrile clean room gloves. See page 3-12 for recommendations.
- Lint-free cloth or paper
- Nut driver, 5.5 mm
- Protective eyewear
- Screwdriver, Phillips #2
- Screwdriver, flat blade
- Wrench, adjustable
- Wrench, hex, 2 mm, 2.5 mm, 3 mm, 4 mm, 5/32-in., 5/64-in., 1/16-in
- Wrench, open-ended, 1/4-in., 5/16-in., 7/16-in. (2), 1/2-in., 9/16-in.
- Wrench, socket, 1/2-in.

Cleaning Stainless Steel Parts

The reagent ion source, ion volume assembly, ion source block, and lenses are made from stainless steel. To clean these parts, follow the procedure described in this topic. Use this procedure with caution because some components can be damaged when exposed to liquids.

The following tools and supplies are needed for cleaning stainless steel parts in the reagent ion source:

- Acetone, analytical grade (or other suitable solvent)
- Aluminum oxide abrasive, number 600[1]
- Applicators, cotton-tipped
- Beaker, 450 mL
- Clean, dry gas
- De-ionized water
- Detergent (Alconox™, Micro-90, or equivalent)
- Dremel™ rotary tool or equivalent (recommended)

[1] Provided in the ETD Accessory Kit.

- Foil, aluminum
- Forceps
- New, white nitrile clean room gloves
- Glycerol, reagent grade
- Lint-free cloth
- Protective eyewear
- Tap water
- Toothbrush, soft
- Ultrasonic cleaner

NOTICE Do not use this procedure to clean ceramic, aluminum, or gold plated parts. See page 6-20 for the method for cleaning ceramic, aluminum, or gold plated parts. ▲

NOTICE Follow the subsequent instructions precisely. If done wrong, the cleaning procedure could damage the ion source lenses. ▲

⚠ CAUTION **Hazardous Chemicals.** Solvents and cleaning agents 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.

❖ To clean reagent ion source stainless steel parts

1. Remove contamination from the surfaces being cleaned:

   a. Use a slurry of number 600 aluminum oxide in glycerol and a cleaning brush or cotton-tipped applicator. Contamination often appears as dark or discolored areas, but might not be visible. The heaviest contamination is usually found around the apertures, such as the electron entrance hole on the ion volume.

   b. Clean each part thoroughly, even if no contamination is visible.

   c. Use the wooden end of an applicator that is cut at an angle to clean the inside corners.

d. Use a Dremel™ tool with the polishing swab at its lowest speed. This will increase the cleaning efficiency and decrease the time required to clean the part.

⚠ CAUTION **Injury Hazard.** To prevent personal injury, keep the Dremel tool away from possible hazards, such as standing water or flammable solvents.

2. Rinse the parts with clean water.
3. Use a clean applicator or toothbrush to remove the aluminum oxide slurry. Do not let the slurry dry on the metal because dried aluminum oxide is difficult to remove.
4. Place the parts in a warm detergent solution in an ultrasonic bath and sonicate them:
   a. Make a solution of detergent and warm tap water in a 400 mL glass beaker.
   b. Use forceps to place the parts in a beaker containing the warm detergent solution.
   c. Place the beaker and contents in an ultrasonic bath for five minutes.
   d. Rinse the parts with tap water to remove the detergent.
5. Sonicate the parts in deionized water:
   a. Use forceps to place the parts in a beaker containing deionized water.
   b. Place the beaker and contents in an ultrasonic bath for five minutes.
   c. If the water is cloudy after sonicating, pour off the water, add fresh water, and place the beaker and its contents in a ultrasonic bath again for five minutes. Repeat until the water is clear.
6. Sonicate the parts in acetone:
   a. Use forceps to place the parts in a beaker containing fresh acetone.
   b. Place the beaker and contents in an ultrasonic bath again for five minutes.
7. Blow-dry the parts immediately. Use clean, dry gas (air or nitrogen) to blow the acetone off the parts.

8. Complete the drying process, doing one of the following:

   - Use forceps to place the parts in a 500 mL glass beaker, cover the beaker with aluminum foil, and put the beaker in an oven set at 100 °C for 30 minutes.

   - Lay the parts on clean aluminum foil (dull side up) and let them dry for 30 minutes.

9. Let the parts cool before you reassemble them.

Cleaning Non-Stainless Steel or Hybrid Parts

To clean the stainless-steel portion of hybrid parts, follow step 1 and step 2 of the instructions on page 6-18. Perform these steps only on the stainless-steel surfaces of hybrid parts. Do not let the aluminum oxide slurry contact the aluminum, ceramic, or gold plated portions of these parts.

⚠ CAUTION **Hazardous Chemicals.** Solvents and cleaning agents 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.

The reagent ion source heater ring, filament spacer, lens holder, and spacers are non-stainless steel parts that are made from aluminum, ceramic, or are gold plated.

❖ **To clean the non-stainless-steel portions of hybrid parts**

1. Scrub all of the parts with a warm detergent solution:

   a. Make a solution of detergent and warm tap water in a 500 mL glass beaker.

   b. Dip a clean cotton-tipped applicator in the detergent mixture and use the applicator to scrub the parts.

      NOTICE Do not soak or sonicate the parts in detergent. ▲

   c. Use forceps to rinse the parts thoroughly with tap water to remove the detergent.

   NOTICE Do not leave aluminum parts, such as the heater ring, in the detergent. Basic solutions, like detergent, damage the surface of aluminum. ▲

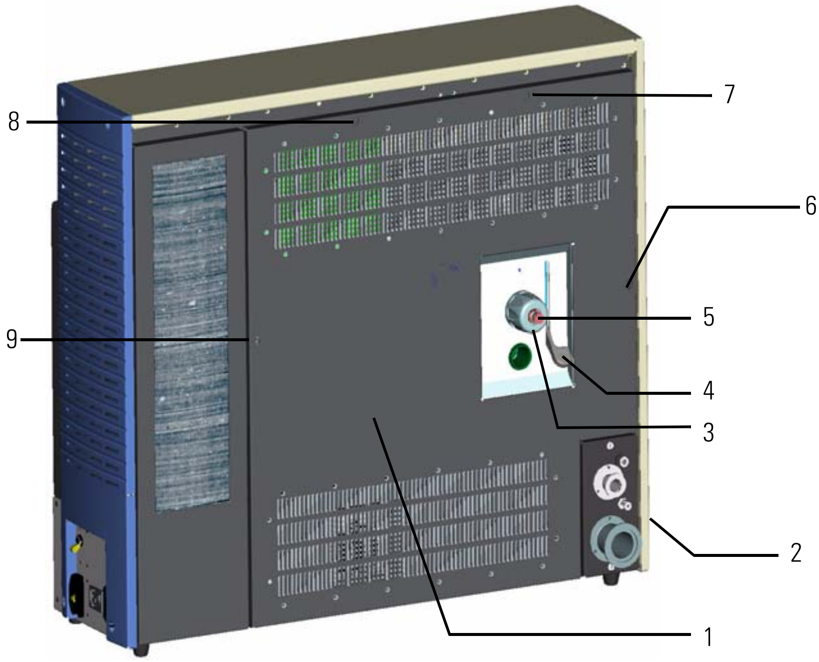
2. Rinse the parts in deionized water. Use forceps to dip the parts in a beaker of deionized water. Change the water if it becomes cloudy. Do not soak or sonicate the parts.

3. Rinse the parts with acetone. Use forceps to dip the parts in a beaker of acetone. Change the acetone if it becomes cloudy. Do not soak or sonicate the parts.

4. Blow-dry the parts immediately. Use clean, dry gas (air or nitrogen) to blow the acetone off the parts.

Removing the Access Panels

During some ETD Module maintenance activities, it is necessary to remove either the ETD main access panel, or the side access panel, or both (see Figure 6-8). Follow the subsequent procedures to remove these panels.



Labeled components: 1=ETD main access panel, 2=side access panel, 3=inlet valve knob, 4=inlet valve lever (down is closed, up is open), 5=inlet valve plug, 6, 7, 8, 9=panel fasteners

Figure 6-8. Rear view of the ETD Module

Removing the ETD Main Access Panel

❖ **To remove the ETD main access panel**

1. Place the ETD Module to Service mode as directed in "Placing the Instrument in Off Condition and Service Mode" on page 6-51.

NOTICE In Service mode, all power to the Orbitrap Elite ETD MS electronics is turned off. There are no user accessible components that carry a voltage in this mode. However, the vacuum pumps continue to operate. ▲

⚠ CAUTION **Burn Hazard.** The reagent vial heaters can be 108 °C (or set point); the transfer line, the restrictor, and the ion source can be at 160 °C. These components might be too hot to touch. Make sure that all of these components are safe to touch before you handle them.

NOTICE The ETD main access panel is interlocked with the ETD Module power. When the ETD main access panel is removed, all power to the ETD Module will be turned off. However, the mechanical pump and turbo pump will continue operating. ▲

2. Remove the inlet valve lever (item 4 in Figure 6-8 on page 6-21) by pulling it down and away from the ETD Module main access panel. Do not rotate the lever upwards. It must remain in its down (closed) position to avoid catastrophic venting of the system.

   NOTICE Rotating the inlet valve lever upwards (to the open position) without the inlet valve plug (item 5 in Figure 6-8) or the ion volume tool in place will cause a catastrophic venting of the system. ▲

3. Unscrew the inlet valve knob (item 3 in Figure 6-8) and remove the inlet valve plug (item 5 in Figure 6-8), the inlet valve knob, and the internal ferrule.
4. Loosen the four panel fasteners (items 6, 7, 8, and 9 in Figure 6-8).
5. The top panel rests on hooks pointing into the upward direction. Tilt the top panel towards you and lift it up and away from the ETD Module.

Removing the ETD Side Access Panel

❖ **To remove the ETD side access panel**

1. If it is not already in Service mode, place the ETD Module in Service mode as directed in “Placing the Instrument in Off Condition and Service Mode” on page 6-51.

NOTICE In Service mode, all power to the Orbitrap Elite ETD MS electronics is turned off. There are no user accessible components that carry a voltage in this mode. However, the vacuum pumps continue to operate. ▲

⚠ CAUTION **Burn Hazard.** The reagent vial heaters can be at 108 °C (or set point). The flow restrictor, the transfer line heaters, and the ion source heater can be at 160 °C. These components might be too hot to touch. Make sure that all of these components are safe to touch before you handle them.

NOTICE The ETD side access panel is interlocked with the ETD Module power. When the ETD side access panel is removed, all power to the ETD Module will be turned off. However, the mechanical pump and turbomolecular pump will continue operating. ▲

2. With a hex wrench, loosen the captive screws at the top and remove the screws at the bottom of gray plastic side panel and remove the panel.

3. With a #2 Phillips screwdriver, loosen the three captive screws on the metal side access panel (item 2 in Figure 6-8 on page 6-21) and remove the panel.

⚠ CAUTION **Burn Hazard.** Reagent vial heaters, ion source heater, flow restrictor, and transfer lines are heated components. They are accessible under the ETD side access panel. Make sure that they are safe to touch before handling them.

Replace the panels by following the above steps in reverse order and reversing the instructions in each step.

Maintenance of the Reagent Ion Source

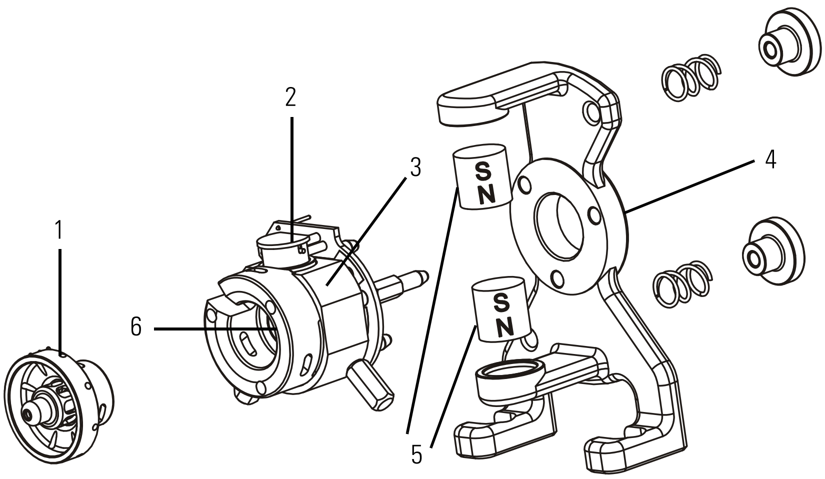
The reagent ion source consists of an ion volume, filament, and ion source lenses. Because the ion volume is exposed directly to samples that are introduced into the reagent ion source, it requires the most frequent cleaning. You can access the ion volume assembly with or without an inlet valve.

To restore system performance, always clean the ion volume first, then the ion source lenses. If cleaning either of these components does not restore system performance, try cleaning the entire reagent ion source.

This section contains these maintenance procedures:

- "Cleaning the Ion Volume With an Inlet Valve" on page 6-24
- "Cleaning the Ion Source Lens Assembly" on page 6-36
- "Cleaning the Ion Source Block" on page 6-42
- "Replacing the Ion Source Filament" on page 6-44
- "Replacing Inlet Valve Components" on page 6-47

The ion source, the ion trap, and their components are shown in Figure 6-9.



Labeled components: 1=ion source lenses, 2=filament assembly, 3=ion source block, 4=magnet support, 5=magnets, 6=ion volume (inside the ion source block, 3)

Figure 6-9. Ion source components (left view)

Cleaning the Ion Volume With an Inlet Valve

The ion volume is where molecules interact with energetic electrons to form ions. Because the ion volume is exposed directly to reagents introduced into the reagent ion source, you will have to clean it more frequently than other parts. How often you have to clean the ion volume assembly will depend on the types and amounts of reagents used.

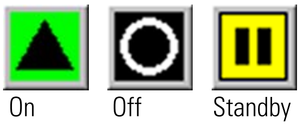
For cleaning the ion volume with an inlet valve, the following tools and supplies are needed:

- Cleaning supplies for stainless steel parts (See "Cleaning Stainless Steel Parts" on page 6-17.)
- Gloves (clean, lint-free, and powder-free)
- Ion volume tool and guide bar

- Lint-free cloth

Use the ion volume tool to access the ion volume by entering the vacuum manifold through the inlet valve without venting the instrument.

❖ To clean the ion volume with an inlet valve



1. Click the On/Standby button in the Tune Plus window to place the Orbitrap Elite ETD mass spectrometer in Standby mode. See Figure 6-10.

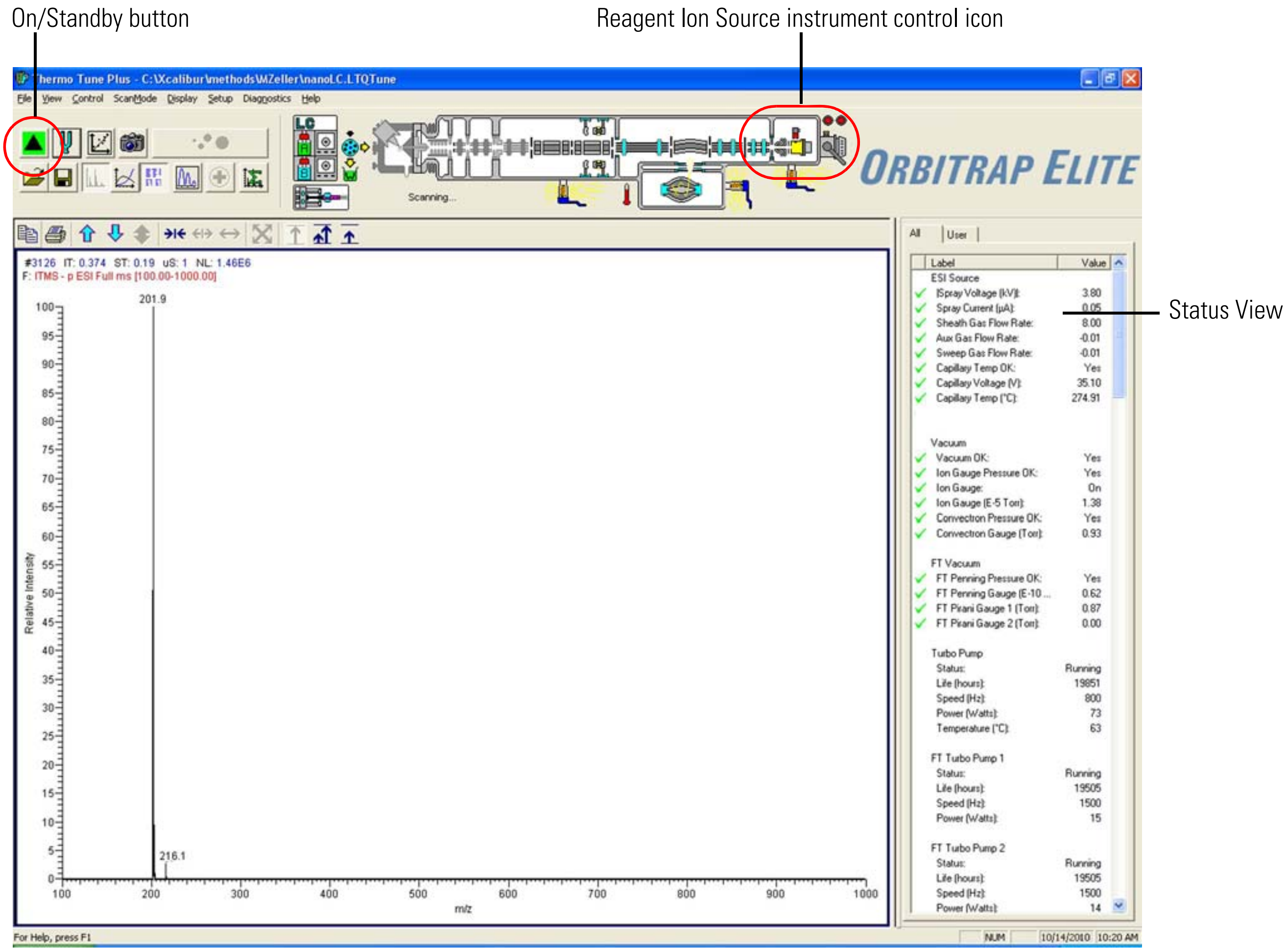
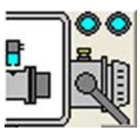
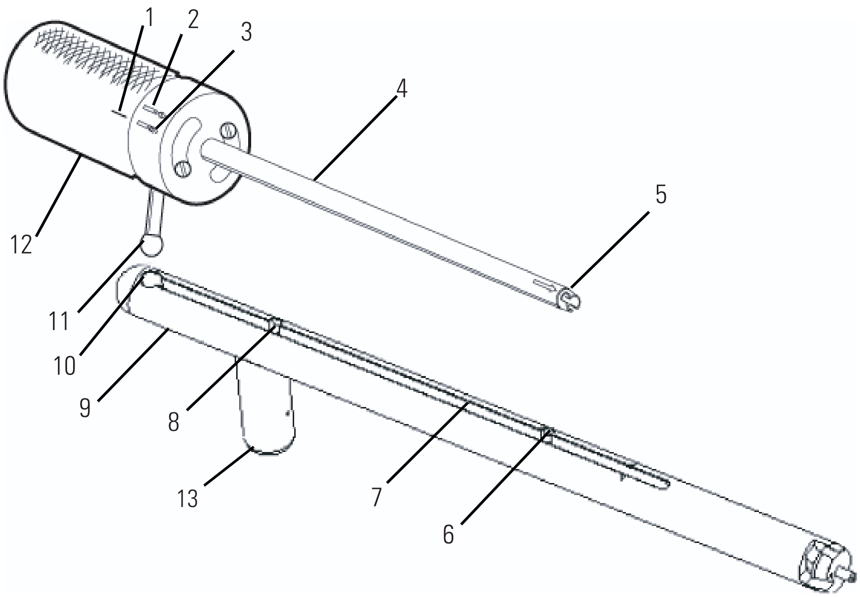


Figure 6-10. Tune Plus window (Orbitrap Elite ETD)



2. Open the Reagent Ion Source dialog box (Figure 6-17 on page 6-29) in Tune Plus by clicking the Reagent Ion Source instrument control icon.
3. Place the guide bar handle (item 13 in Figure 6-11) to the 3 o'clock position (Figure 6-12 on page 6-26).



Labeled components: 1=alignment line, 2=lock position, 3=unlock position, 4=ion volume tool, 5=bayonet lock, 6=second stop, 7=guide ball track, 8=first stop, 9=guide bar, 10=guide ball hole, 11=guide ball, 12=ion volume tool handle, 13=guide bar handle

Figure 6-11. Ion volume tool components

4. Insert the guide bar (item 9 in Figure 6-11) into the guide bar opening in the back of the ETD Module (Figure 6-12).

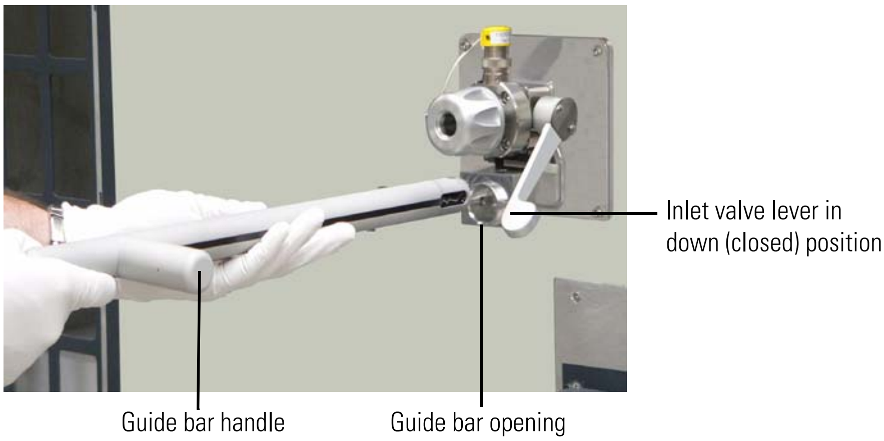


Figure 6-12. Guide bar being inserted into guide bar opening[a]

[a] Guide bar handle is facing to the right. The inlet valve is closed when the inlet valve lever is in the down position and open when it is in the up position.

5. Push the guide bar in as far as it will go, then rotate it 90° clockwise to lock in the guide bar (Figure 6-13). The guide bar handle faces the floor at the completion of this step.

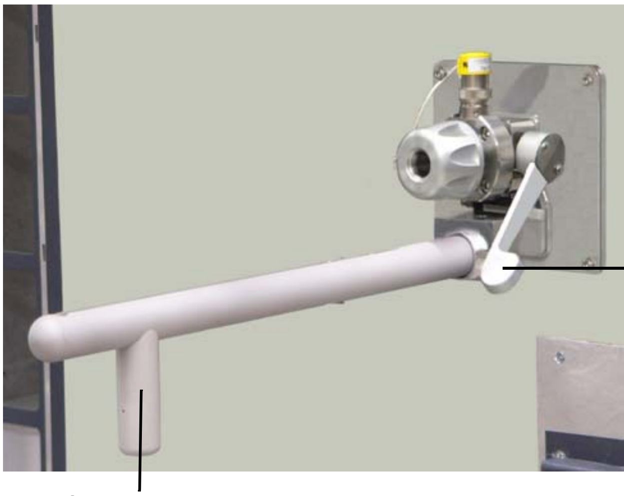
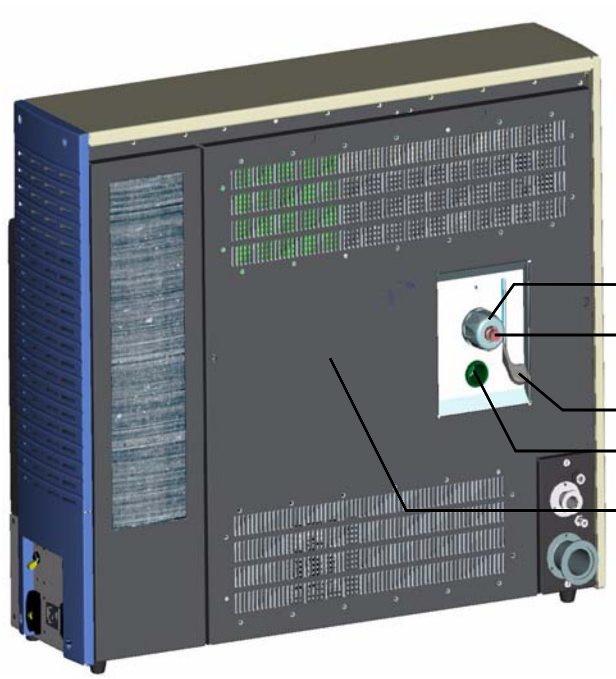


Figure 6-13. Guide bar insertion complete[a]

[a] Guide bar handle is facing the floor. The inlet valve is closed when the inlet valve lever is in the down position and open when it is in the up position.

6. Prepare the inlet valve and ion volume tool for insertion.



Labeled components: 1=inlet valve knob, 2=inlet valve plug, 3=inlet valve lever (down is closed, up is open), 4= guide bar opening, 5=main access panel

Figure 6-14. Rear view of the ETD Module, showing the inlet valve

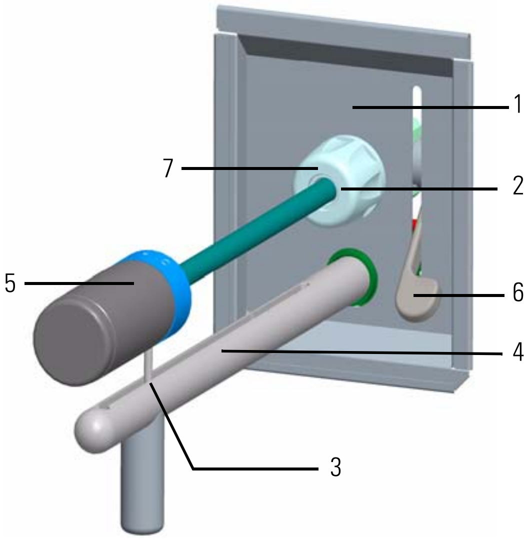
Make sure that the inlet valve is closed (inlet valve lever is down, as shown in Figure 6-13) and remove the inlet valve plug (item 2 in Figure 6-14). Do this by rotating (loosening) the inlet valve knob (item 1 in Figure 6-14) until the inlet valve plug will slide out easily. The inlet valve plug prevents air from entering the vacuum manifold if the inlet valve is inadvertently opened.

7. Turn the ion volume tool handle to the unlock position, which indicates that the ion volume tool is in position to accept the ion volume. See Figure 6-15.

Figure 6-15. Ion volume tool handle in the unlock position

8. Insert the ion volume tool and evacuate the inlet valve:

   a. Insert the guide ball into the guide ball hole.



Labeled components: 1=ion volume tool entry housing, 2=inlet valve opening, 3=first stop, 4=guide bar, 5=ion volume tool, 6=inlet valve lever, 7=inlet valve knob

Figure 6-16. Ion volume tool guide bar first stop

b. Slide the ion volume tool forward in the guide bar track until the guide ball is at the guide bar's first stop, which is shown in Figure 6-11 on page 6-26 and Figure 6-16.

c. Slide the ion volume tool so the guide ball is in the groove at the first stop (Figure 6-11 and Figure 6-16). This prevents the probe from being pulled forward when the inlet valve is evacuated.

d. Tighten the inlet valve knob (Figure 6-16) to ensure that a leak-tight seal is made.

e. Click **Open Probe Interlock** in the Reagent Ion Source dialog box (Figure 6-17). A message box appears that tells you that the probe interlock is being pumped down. The target pressure is <0.1 mTorr. If a pressure of 0.1 mTorr or less is not obtained, replace the inlet valve seal as described in "Replacing Inlet Valve Components" on page 6-47. When the target pressure is achieved, a message appears that tells you that the ball valve can be opened (Figure 6-18).

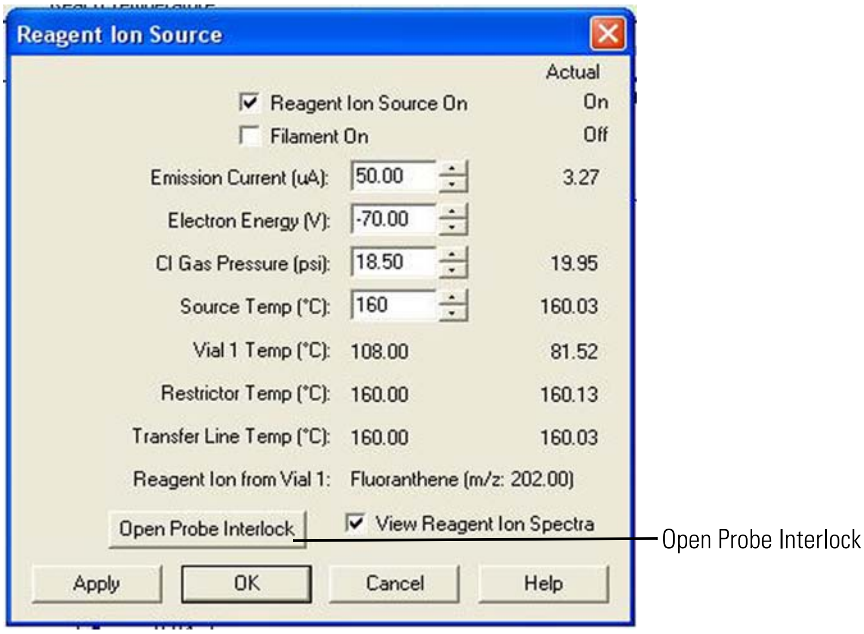


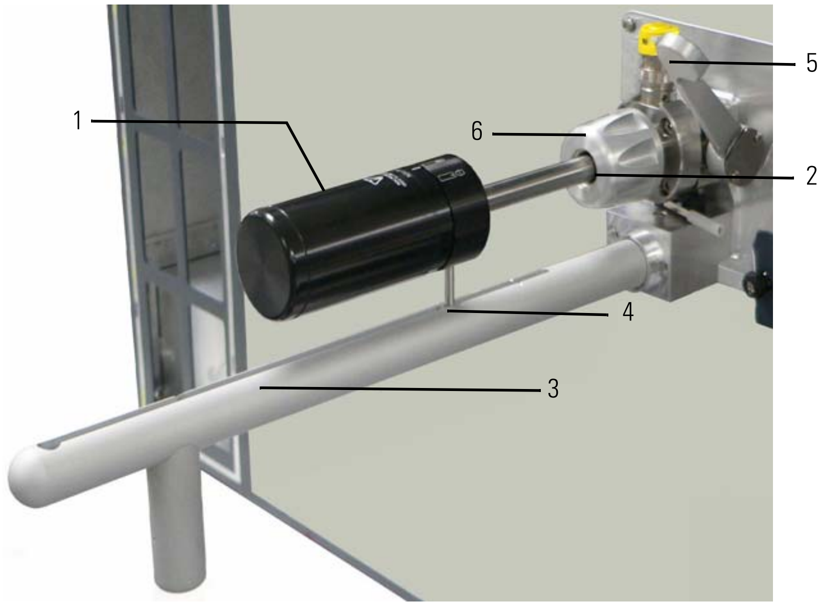
Figure 6-17. Reagent Ion Source dialog box, Open Probe Interlock button.

Figure 6-18. Instrument Message box: The Ball Valve can now be opened

f. When evacuation is complete, push up the inlet valve lever to open the inlet valve (Figure 6-19).

9. Remove the ion volume:

   a. Slide the ion volume tool into the vacuum manifold until the tip of the ion volume tool is fully inserted into the ion volume holder, as shown in Figure 6-19.



Labeled components: 1=ion volume tool, 2=inlet valve opening, 3=guide bar, 4=second stop, 5=inlet valve lever in open (up) position, 6=inlet valve knob

Figure 6-19. Ion volume tool inserted into the inlet valve

Figure 6-20. Detail of ion volume tool fully inserted into the inlet valve

You will know that the ion volume tool is fully inserted into the ion volume holder because the guide ball (item #11, Figure 6-11 on page 6-26) will be just past the first mark on the guide bar as shown in Figure 6-20 on page 6-30.

b. Turn the ion volume tool handle counterclockwise to the lock position, See Figure 6-21. An audible click indicates that the handle is fully engaged in the lock position and is holding the ion volume.

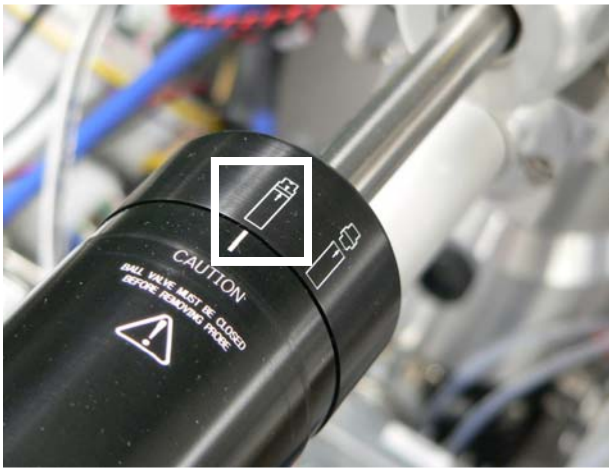


Figure 6-21. Ion volume tool handle in the locked position

c. Withdraw the ion volume tool (the ion volume is attached) until the guide ball reaches the first stop (see Figure 6-11 on page 6-26 and Figure 6-16 on page 6-28 for the first stop position).

d. Close the inlet valve by pushing the lever down.

NOTICE Do not withdraw the ion volume tool beyond the point where the guide ball reaches the first stop in the guide bar. Close the inlet valve before you withdraw the ion volume tool past the first stop. Otherwise, the system will vent to the atmosphere and cleaning the components that are under vacuum will be required. ▲

e. Loosen the inlet valve knob (Figure 6-19 on page 6-30).

f. Continue withdrawing the ion volume tool completely from the inlet valve by sliding the ion volume tool through the guide ball track in the guide bar.

⚠ CAUTION **Burn Hazard.** The ion volume will be too hot to touch. Let it cool to room temperature before you handle it.

10. Clean the ion volume:

   a. Turn the ion volume tool handle to the unlock position (Figure 6-15 on page 6-28). The ion volume tool handle unlock position icon is shown at the left.

   b. Remove the ion volume from the ion volume tool. Using clean gloves, press the ion volume into the tip of the ion volume tool and rotate it to disconnect the bayonet pins from the pin guides. Pull the ion volume out of the ion volume tool, as illustrated in Figure 6-22.

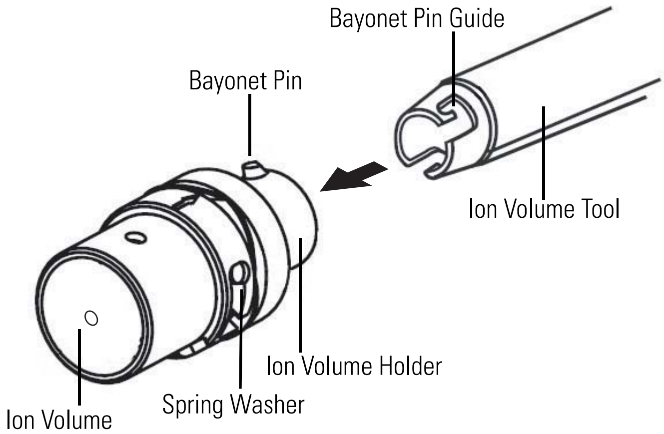


Figure 6-22. Ion volume assembly

   c. Press the ion volume into the ion volume holder and rotate the ion volume to remove it from the ion volume holder See Figure 6-23.

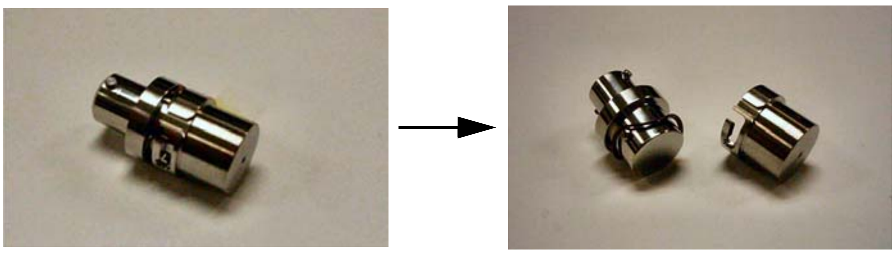


Figure 6-23. Separating ion volume and ion volume holder

   d. Clean ion volume and ion volume holder according to the instructions in "Cleaning Stainless Steel Parts" on page 6-17.

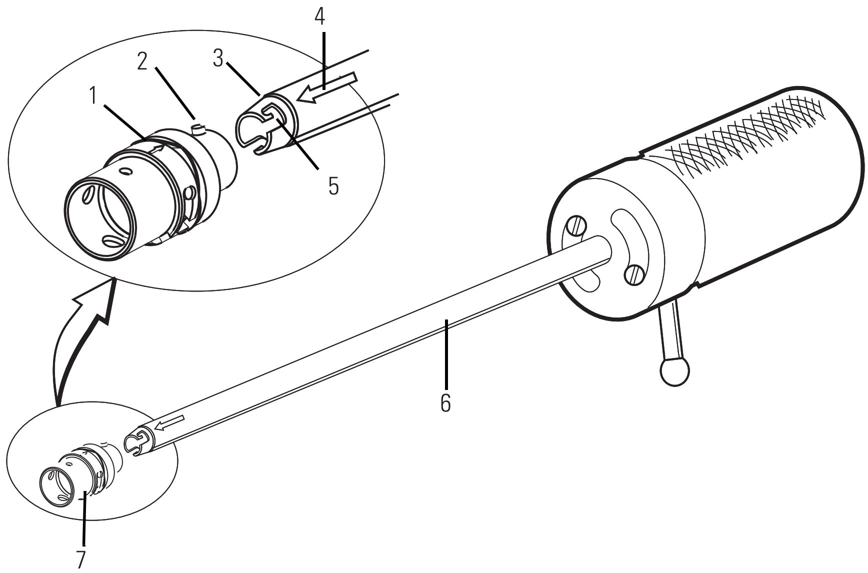
❖ **To reinsert the ion volume**

1. Press the ion volume into the ion volume holder and rotate the ion volume to secure it to the ion volume holder.

2. Place the clean ion volume on the ion volume tool:

   a. Place the ion volume into the bayonet lock located on the ion volume tool. Make sure that the alignment arrows on the ion volume and ion volume tool are facing each other. See Figure 6-24.

   NOTICE To avoid damage to the ion source, make sure that the arrows on the ion volume tool and ion volume are aligned. ▲



Labeled components: 1=ion volume alignment arrow, 2=bayonet pin, 3=bayonet lock, 4=ion volume tool alignment arrow, 5=bayonet guide, 6=ion volume tool, 7=ion volume

Figure 6-24. Placing the ion volume on the ion volume tool

   NOTICE Wear clean, lint-free, and powder-free gloves when you handle parts inside the vacuum manifold. ▲

   b. Turn the ion volume tool handle to the lock position. (See Figure 6-21 on page 6-31.)

3. Insert the ion volume tool and evacuate the inlet valve:

   a. Insert the guide ball into the guide ball hole and slide the ion volume tool forward in the guide bar track until the guide ball is at the guide bar's first stop (see Figure 6-11 on page 6-26 and Figure 6-16 on page 6-28).

   b. Turn the ion volume tool so that the guide ball is in the groove at the first stop (Figure 6-16 on page 6-28). This prevents the probe from being pulled forward when the inlet valve is evacuated.

c. Tighten the inlet valve knob to ensure a leak-tight seal (Figure 6-19 on page 6-30).

d. Click **Open Probe Interlock** in the Reagent Ion Source dialog box (Figure 6-17 on page 6-29). A message box will appear stating that the probe interlock is being pumped down. The target pressure is <0.1 mTorr. If a pressure of 0.1 mTorr or less is not obtained, the inlet valve seal must be replaced as described in "Replacing Inlet Valve Components" on page 6-47. When the target pressure is achieved, a message will appear stating that the ball valve can be opened. See Figure 6-18 on page 6-29.

e. When evacuation is complete, push the inlet valve lever up to open the inlet valve. See Figure 6-19 on page 6-30.

4. Reinsert the ion volume:

a. Slide the ion volume tool into the vacuum manifold, as illustrated in Figure 6-19.

b. Listen for a click indicating that the ion volume has connected with the ion source block. The guide ball will be slightly beyond the second stop on the guide bar. See Figure 6-20 on page 6-30.

c. Turn the ion volume tool handle to the unlock position. See Figure 6-25.

Figure 6-25. Ion volume tool handle in the unlock position

i. Withdraw the ion volume tool away from the ion volume about 2.5 cm (1 in) and turn the ion volume tool handle to the lock position. See Figure 6-26 on page 6-35.

ii. Slide the ion volume tool back into the vacuum manifold until the end of the ion volume tool just touches the ion volume.

iii. If the ion volume tool does not go into the inlet valve completely, the ion volume is not seated properly.

d. Withdraw the ion volume tool until the guide ball reaches the first stop (see Figure 6-11 on page 6-26 and Figure 6-16 on page 6-28).

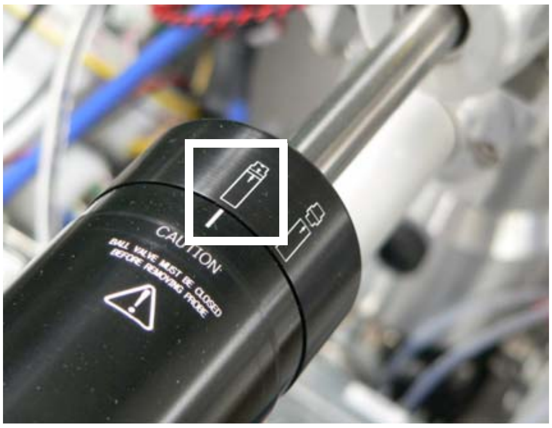


Figure 6-26. Ion volume tool handle in the locked position

e. Close the inlet valve by pushing down on the inlet valve lever (Figure 6-14 on page 6-27).

NOTICE Do not withdraw the ion volume tool beyond the point where the guide ball reaches the first stop in the guide bar. Close the inlet valve before you withdraw the ion volume tool past the first stop. Otherwise, the system vents to the atmosphere. ▲

f. Loosen the inlet valve knob (item 6 in Figure 6-19 on page 6-30).

g. Continue withdrawing the ion volume tool completely from the inlet valve by sliding the ion volume tool through the guide ball track in the guide bar.

5. Remove the ion volume tool and guide bar from the vacuum manifold:

   a. Remove the guide bar by rotating it 90° counterclockwise and sliding it out of the entry housing.

   b. Replace the inlet valve plug and tighten the inlet valve knob (item 6 in Figure 6-19 on page 6-30).

   c. Click **Close** in the message stating that the ball valve can be opened. (See Figure 6-18 on page 6-29.)

6. Re-tune the mass spectrometer.

NOTICE Tune Plus provides an evaluation procedure for CI gas pressure under **Diagnostics > Diagnostics > Tools > System evaluation > Reagent CI gas pressure evaluation**. Thermo Fisher Scientific recommends that you perform this procedure after you have replaced the filament and/or the ion volume. ▲

Cleaning the Ion Source Lens Assembly

If cleaning the ion volume did not restore system performance, try cleaning the ion source lens assembly. The ion source lens assembly comes in direct contact with reagent ions that are introduced into the ETD Module and needs to be cleaned periodically (though not as often as the ion volume).

❖ **To clean the ion source lens assembly**

1. Prepare the ETD Module for maintenance:

   a. Prepare a clean work area by covering the area with a clean lint-free cloth.

   b. Shut down and vent the ETD Module. (See "Shutting Down the Instrument" on page 5-7.)

   NOTICE Shut down and unplug the Orbitrap Elite ETD mass spectrometer before you proceed with the next steps of this procedure. ▲

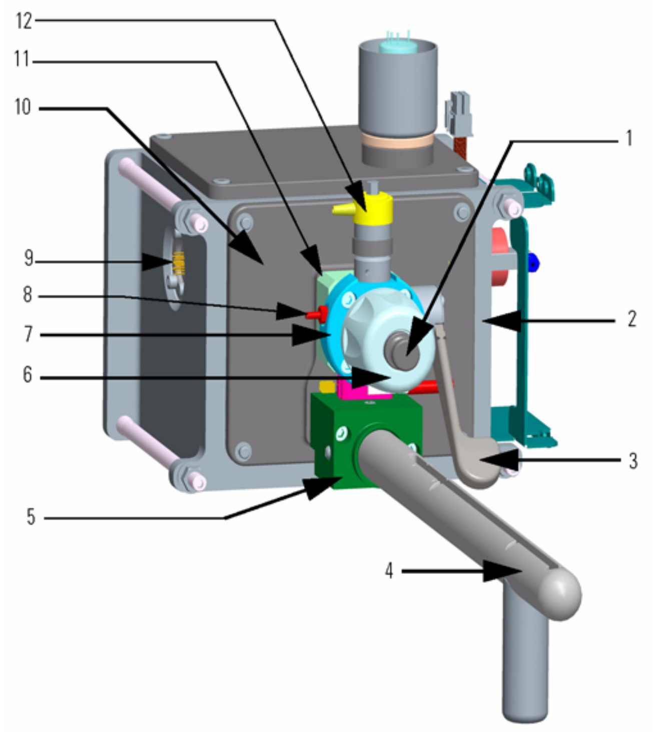
   NOTICE Wear clean, lint- and powder-free gloves when you handle parts inside the vacuum manifold. ▲

⚠ CAUTION **High Temperatures.** Burn Hazard. The ion source might be too hot to touch even if the cooling nitrogen has completed its cycle. Make sure that the ion source has cooled to room temperature before you handle it.

2. Remove the ion source assembly:

   a. Remove the main access panel of the ETD Module (item 1 in Figure 6-8 on page 6-21). Follow the procedures in "Removing the ETD Main Access Panel" on page 6-21.

      NOTICE It is good practice to keep the inlet valve lever in the down (closed) position when it is not explicitly required to be in the up position (open), even if the vacuum manifold is at atmospheric pressure. This is to be consistent with maintenance procedures that rely on the inlet valve lever being closed at the appropriate step to prevent the accidental loss of vacuum. If the vacuum is accidentally lost the system might be damaged. At a minimum, the components that were under vacuum might have to be cleaned. ▲



Labeled components: 1=inlet valve plug, 2=vacuum manifold, 3=inlet valve lever, 4=guide bar, 5=entry housing, 6=inlet valve knob, 7=inlet valve block, 8=foreline hose connection, 9=12 pin feedthrough, 10=vacuum manifold probe plate, 11=ball valve housing, 12= inlet valve solenoid

Figure 6-27. Inlet valve components (ion volume tool not shown)

b. Remove all connectors between the components on the vacuum manifold probe plate (item #10, Figure 6-27 on page 6-37) and the ETD Control PCB (Figure 2-3 on page 2-22).

c. Remove the valve shield from the vacuum manifold probe plate (Figure 6-28) by loosening the four screws at the corners of the shield.

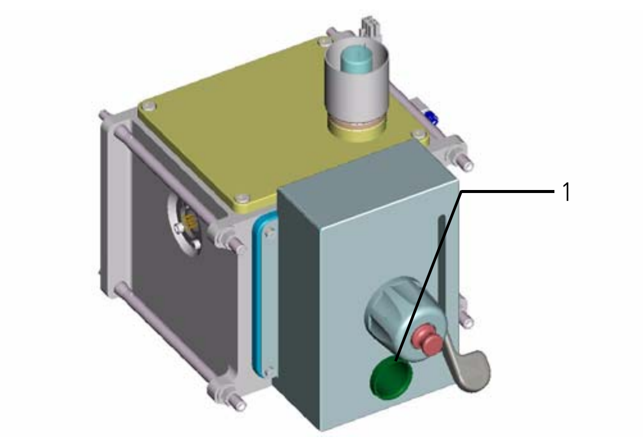


Figure 6-28. Valve shield (1) covering the vacuum manifold probe plate

d. Remove the foreline hose on the source from its connection (Figure 6-29 and item 8 in Figure 6-27).

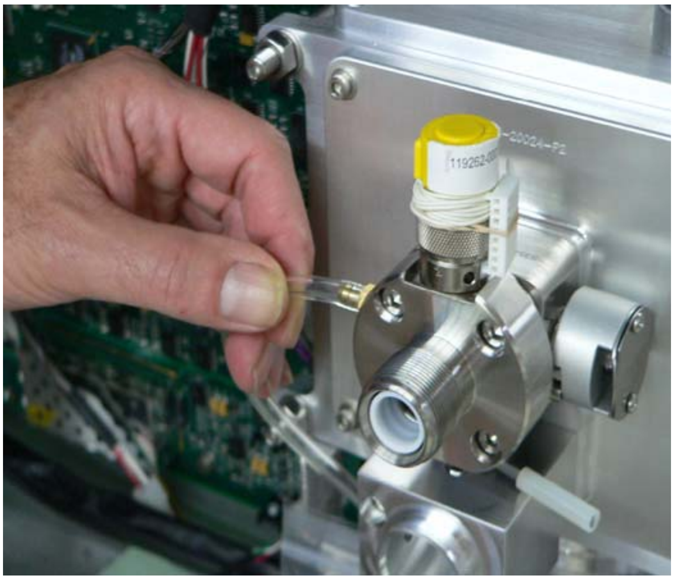


Figure 6-29. Removing the foreline hose from its connection

e. Remove the four screws holding the vacuum manifold probe plate (Figure 6-30 and item 10 in Figure 6-27 on page 6-37). Support the plate with your hand as shown in Figure 6-30. Arrows point to the four hex screw locations (items 1–4).

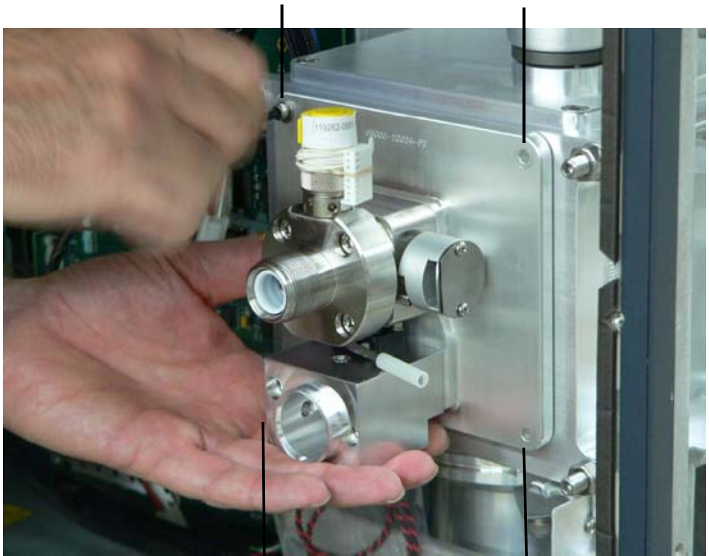


Figure 6-30. Unscrewing the vacuum manifold probe plate

f. Remove the vacuum manifold probe plate (Figure 6-31).

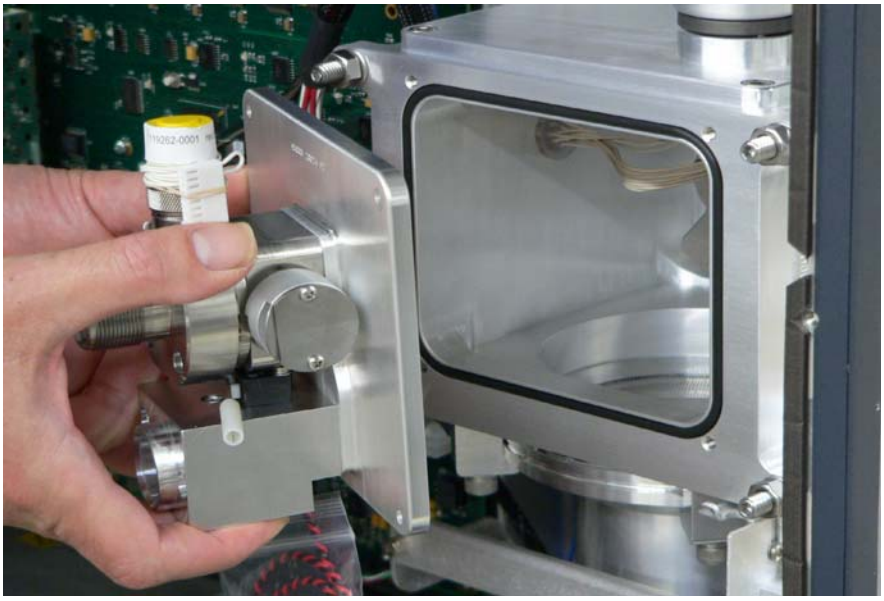
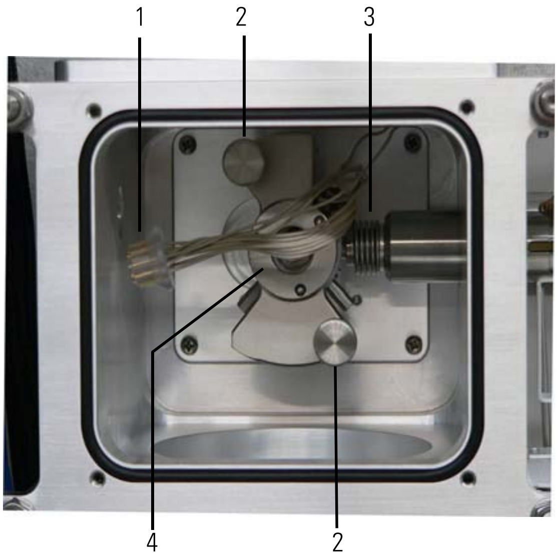


Figure 6-31. Removing the vacuum manifold probe plate

g. Unplug the 12-pin feedthrough harness from the feedthrough (Figure 6-32).



Labeled components: 1=unplugged 12 pin feedthrough, 2=thumbscrews, 3=transfer line bellows, 4=ion source assembly

Figure 6-32. Interior of vacuum manifold

h. Remove the ion source assembly from the vacuum manifold (Figure 6-33 on page 6-40) by first loosening the ion source thumbscrews (item 2 in Figure 6-32).

i. Second, as you remove the ion source assembly (item 1 in Figure 6-33) gently shift it to the left (arrow 2 in Figure 6-33) before and while pulling it out. This will allow the ion source assembly to disengage from the transfer line bellows (item 3 in Figure 6-33) as it is removed. Or, gently depress the transfer line bellows (Figure 6-32) to disengage it from the ion source assembly.

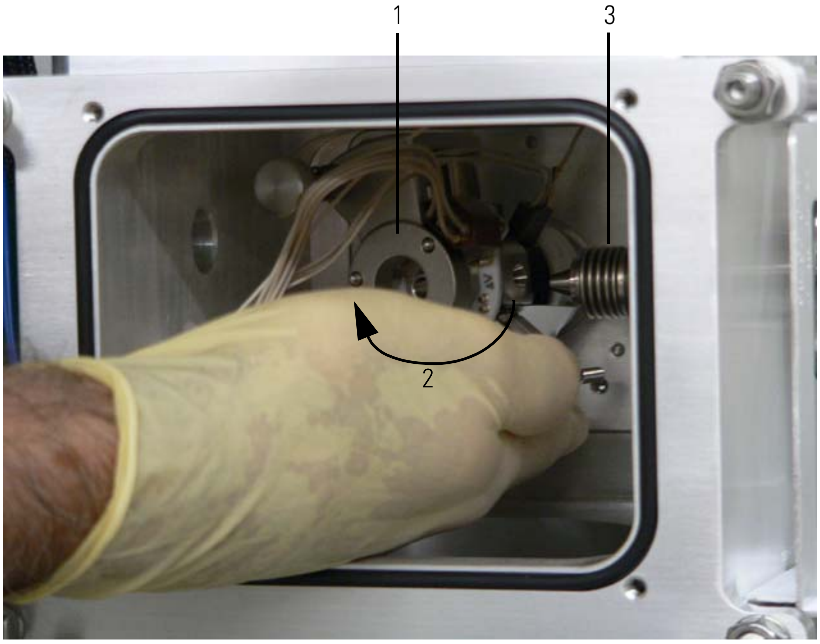
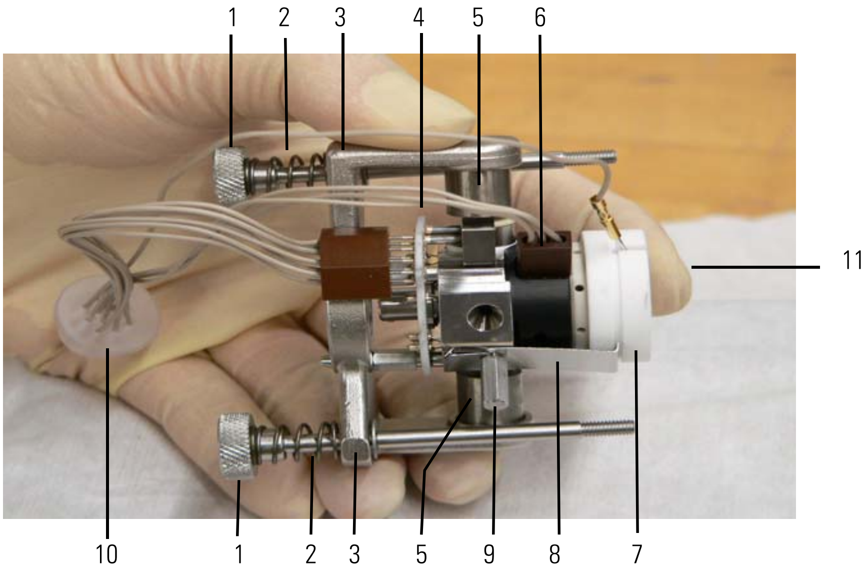


Figure 6-33. Removing the ion source assembly from the vacuum manifold[a]

[a] The ion source assembly (item 1) is gently shifted to the left (arrow 2) to allow the ion source assembly to disengage from the transfer line bellows (item 3) as it is removed.

The ion source assembly is held together with a clip (item 8 in Figure 6-34 on page 6-41). However, it is necessary to keep the tips of your gloved fingers on both the front edge of the ceramic lens holder (item 11 in Figure 6-34) and the back of the magnet yoke (item 3 in Figure 6-34) when you handle the ion source assembly. This prevents unsecured components inside of the ceramic lens holder from falling out.

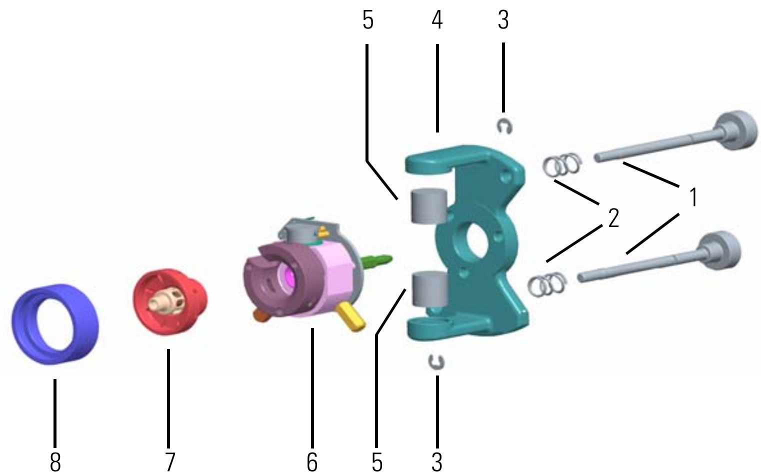
NOTICE When you handle the ion source assembly, use gentle finger pressure on each end (as instructed above) to keep unsecured components from falling out of the assembly. ▲



Labeled components: 1=thumbscrew, 2=springs, 3=magnet yoke, 4=Ion Source PCB, 5=magnets, 6=ion source block, 7=ceramic lens holder, 8=spring clip, 9=spring clip thumb screw, 10=12 pin feedthrough harness, 11=finger over front edge of ceramic lens holder to keep unsecured components from falling out of the ion source assembly.

Figure 6-34. Ion source assembly

An exploded view of the ion source assembly is shown in Figure 6-35.



Labeled components: 1=thumbscrews, 2=springs, 3=E-clips , 4=magnet yoke, 5=magnets, 6=ion source, 7=ion source lens assembly, 8=ceramic lens holder

Figure 6-35. Ion source assembly exploded view

3. Separate the magnet yoke and the ion source.

4. Remove the ion source lens assembly from the ceramic lens holder (Figure 6-35).

5. Clean the ion source lens assembly according to the procedure in "Cleaning Stainless Steel Parts" on page 6-17. Pay particular attention to the areas inside the tube and around the holes in the lens assembly.

6. Replace the ion source assembly:

   a. Insert the lens assembly into the ceramic lens holder.

   b. Reassemble the ion source assembly.

   c. Reinstall the ion source assembly into the vacuum manifold by following step 2 in reverse order.

7. Restore the ETD Module to operational status. See "Starting up the System after a Shutdown" on page 5-9.

Cleaning the Ion Source Block

If cleaning the ion volume and ion source lens assembly does not restore system performance, you may need to clean the ion source block. Generally, you need to clean the ion source block no more than once every six months.

Supplies needed for cleaning the ion source:

- Cleaning supplies
- Gloves (clean, lint-free, and powder-free)
- Lint-free cloth

❖ **To clean the ion source block**

1. Prepare the ETD Module for maintenance:

   a. Prepare a clean work area by covering the area with lint-free cloth.

   b. Shut down and vent the Orbitrap Elite ETD mass spectrometer. (See "Shutting Down the Orbitrap Elite Mass Spectrometer Completely" on page 5-7.)

   NOTICE Shut down and unplug the Orbitrap Elite ETD MS before you continue with the next steps of this procedure. ▲

c. Remove the ion source assembly by following the procedures in step 2 in "Cleaning the Ion Source Lens Assembly" on page 6-36.

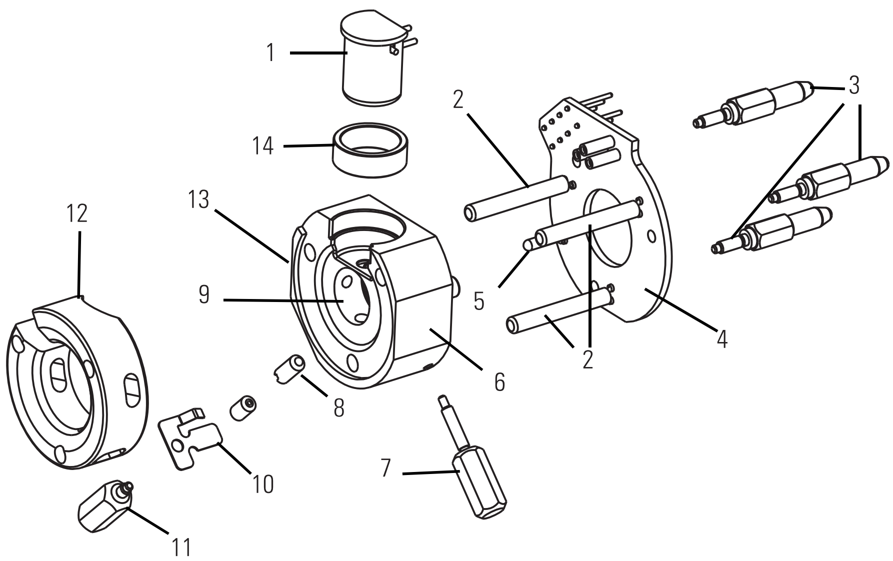
NOTICE Wear clean, lint- and powder-free gloves when you handle parts inside the vacuum manifold. ▲

2. Disassemble the ion source assembly (Figure 6-34 on page 6-41 and Figure 6-35 on page 6-41), remove and disassemble the ion source (Figure 6-36):

   a. Remove the magnet yoke and the ion source block with the ion source lens assembly.

   b. Remove the ion source lens assembly.

   c. Remove the ion source.



Labeled components: 1=ion source filament, 2=cartridge heaters, 3=base studs (3×), 4=Ion Source PCB, 5=temperature sensor, 6=ion source block, 7=ion volume key thumbscrew, 8=ion volume pin, 9=ion volume, 10=spring clip, 11=spring clip thumb screw, 12=heater ring, 13=sample inlet aperture (in side of item 6), 14=ceramic spacer

Figure 6-36. Ion source, exploded view

   d. Remove the three base studs (item 3 in Figure 6-36). Be careful not to damage the leads on the Ion Source PCB (item 4 in Figure 6-36).

   e. Gently remove the Ion Source PCB (item 4 in Figure 6-36) from the ion source:

      i. Loosen the spring clip thumbscrew (item 11 in Figure 6-36) and the spring clip (item 10 in Figure 6-36).

ii. Slide the three cartridge heaters and the temperature sensor (items 2 and 5 in Figure 6-36) off the ion source.

iii. Pull the filament (item 1 in Figure 6-36) straight away from the three filament connectors on the Ion Source PCB. Do not bend or twist the cartridge heaters or the temperature sensor.

f. Remove the filament and ceramic spacer (items 15 and 1 in Figure 6-36) from the ion source block (item 6 in Figure 6-36).

g. Remove the ion volume key thumbscrew (item 7 in Figure 6-36).

NOTICE It is not necessary to remove the ion volume pin (item 8 in Figure 6-36). If you remove it, you should reinsert it just far enough so the ball will keep an ion volume (item 9 in Figure 6-36) from falling out. If the ball extends too far, the ion volume will be difficult to remove. ▲

3. Clean the ion source parts and replace the ion source assembly:

   a. Clean each component of the ion source, as described in "Cleaning Stainless Steel Parts" on page 6-17 and "Cleaning Non-Stainless Steel or Hybrid Parts" on page 6-20.

   b. Reassemble the ion source block.

   c. Reassemble the ion source assembly.

   d. Reinstall the ion source assembly into the vacuum manifold by following step 2 of "Cleaning the Ion Source Lens Assembly" on page 6-36 in reverse order.

4. Restore the ETD Module to operational status. See "Starting up the System after a Shutdown" on page 5-9.

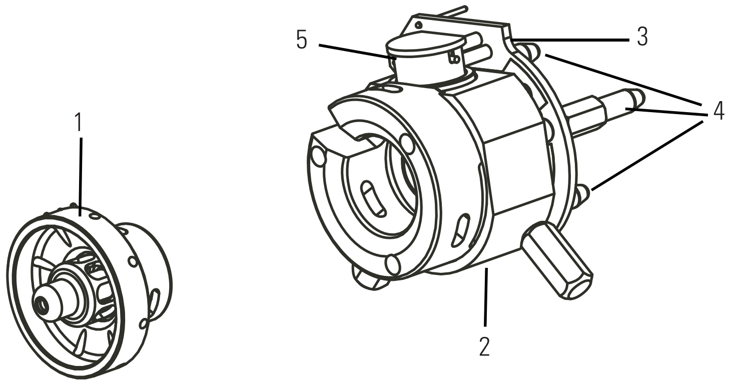
Replacing the Ion Source Filament

The number of ions produced in the ion source is approximately proportional to the filament emission current. If you notice that ion production is low, this might indicate that the filament has failed and needs to be replaced. If the measured emission current is substantially less than the value that the emission current is set to, or if the measured emission current is decreasing over time, then the filament has failed or is failing and needs to be replaced. The ion source filament assembly is shown in Figure 6-37 on page 6-45.

Supplies needed for replacing the ion source filament:

- Filament Assembly DSQ II

- Gloves, clean, lint-free, and powder-free
- Protective eyewear
- Lint-free cloth
- Forceps or dental pick



Labeled components: 1=ion source lens assembly, 2=ion source block, 3=Ion Source PCB, 4=base studs (3x), 5=ion source filament

Figure 6-37. Ion source lens assembly and ion source

❖ **To replace the ion source filament**

1. Prepare the ETD Module for maintenance:

   a. Prepare a clean work area by covering the area with lint-free cloth.

   b. Shut down and vent the Orbitrap Elite ETD mass spectrometer. (See "Shutting Down the Orbitrap Elite Mass Spectrometer Completely" on page 5-7.)

   NOTICE Shut down and unplug the Orbitrap Elite ETD MS before proceeding with the next steps of this procedure. ▲

   c. Remove the ion source assembly by following the procedures in step 2 in "Cleaning the Ion Source Lens Assembly" on page 6-36.

   NOTICE Wear clean, lint- and powder-free gloves when you handle parts inside the vacuum manifold. ▲

2. Disassemble the ion source assembly (Figure 6-34 on page 6-41 and Figure 6-35 on page 6-41), remove and disassemble the ion source (Figure 6-36 on page 6-43):

   a. Remove the ion source lens assembly (item 1 in Figure 6-37).

b. Remove the three base-studs (item 3 in Figure 6-36, item 4 in Figure 6-37).

c. Remove the filament assembly (items 1 and 15 in Figure 6-36, item 5 in Figure 6-37) and ion source block (item 2 in Figure 6-37) from the three filament connectors and cartridge heaters (item 2 in Figure 6-36) on the Ion Source PCB (item 4 in Figure 6-36) according to the procedure in step e of "Cleaning the Ion Source Block" on page 6-43.

NOTICE Now is a good time to clean the ion volume and ion source lenses. ▲

3. Inspect and install a new filament assembly:

a. Turn the filament assembly over and, using a strong light and a magnifying glass, make sure that the filament wire is centered in the electron lens hole. If necessary, carefully use forceps (or a dental pick) to adjust the filament wire. Figure 6-38 shows the centered filament wire as seen from the bottom of the filament through the electron lens hole.

NOTICE A bent filament can lead to a low or absent anion signal. If the filament wire is bent, not centered, or otherwise damaged, you must replace the filament assembly. ▲

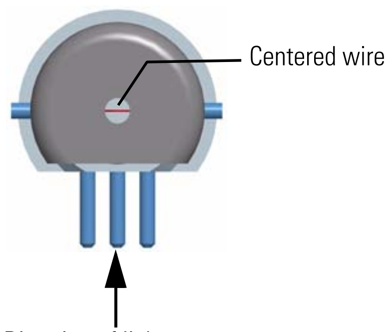


Figure 6-38. Filament wire as seen from the bottom of the filament through the electron lens hole

b. Insert the filament into the ceramic spacer of the ion source block (item 14 in Figure 6-36 on page 6-43).

c. Align the filament leads with the Ion Source PCB connectors and gently press the leads into the connectors. Normally, there is a small gap (about 0.020 in or 0.50 mm) between the filament and the connectors. The gap allows the ceramic filament centering ring (spacer) to properly position and align the electron lens hole with the ion volume.

d. Reinstall the three base-studs (item 3 in Figure 6-36, item 4 in Figure 6-37 on page 6-45).

4. Reassemble ion source and ion source assembly.

5. Insert the ion source assembly into the vacuum manifold.

6. Restore the ETD Module to operational status. See "Starting up the System after a Shutdown" on page 5-9.

NOTICE Tune Plus provides an evaluation procedure for CI gas pressure under **Diagnostics > Diagnostics > Tools > System evaluation > Reagent CI gas pressure evaluation**. Thermo Fisher Scientific recommends performing this procedure after replacing the filament and/or the ion volume. ▲

Replacing Inlet Valve Components

Replace the inlet valve components when the inlet valve seal or the inlet valve is being replaced.

Tools and supplies needed for replacing inlet valve components:

- Inlet Valve Seal Kit
- Lint-free cloth
- Wrench, open-ended, 5/16-in
- Wrench, hex, 4 mm

❖ **To replace inlet valve components**

1. Pull down the inlet valve lever to close the inlet valve. See Figure 6-39.

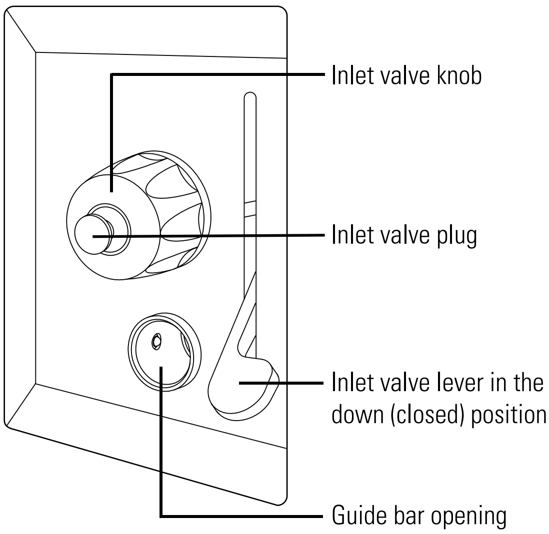


Figure 6-39. Inlet valve components

2. Rotate the inlet valve knob counterclockwise until you can easily remove the inlet valve plug.

3. Continue to rotate the valve knob until you can remove it.

   The inlet valve knob has a stainless-steel ferrule inside. Keep the inlet valve knob and ferrule together.

4. Pull out the knob on the inlet valve seal tool[1], so that the knob is loose. See Figure 6-40.

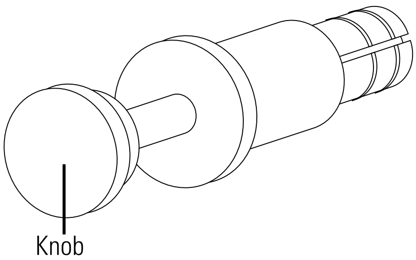


Figure 6-40. Inlet valve seal tool

5. Insert the tool straight into the inlet valve. See Figure 6-41.

[1] Item contained in Inlet Valve Seal Kit.

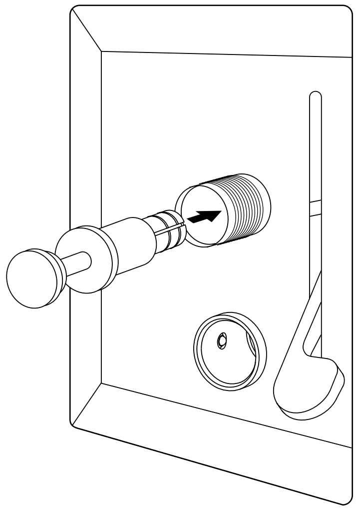


Figure 6-41. Inlet valve seal tool inserted in the inlet valve

NOTICE Do not scratch the surface of the seal. Use only the inlet valve seal tool to remove or install an inlet valve seal. ▲

6. Press in the knob on the tool until it stops.
7. Remove the tool. The inlet valve seal should be on the tool. See Figure 6-42.

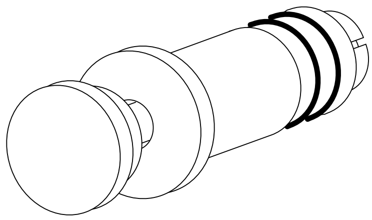


Figure 6-42. Inlet valve seal on the inlet valve seal tool

8. Loosen the knob to disengage the seal. See Figure 6-43.

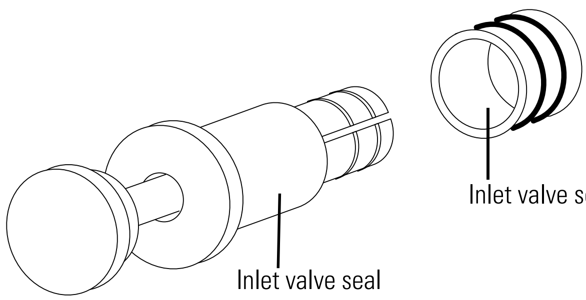


Figure 6-43. Inlet valve seal disengaged from tool

9. Discard the seal with its O-rings in place.

10. Place one O-ring[1] into each of the two slots on the inlet valve seal[1].
11. Put the new inlet valve seal onto the inlet valve seal tool.
12. Insert the inlet valve seal tool into the inlet valve into it stops.
13. Remove the tool. The O-rings on the valve seal secure the inlet valve seal in the opening.
14. Reinstall the ferrule, knob, and plug into the inlet valve opening.

Replacing the Reagent Vials

A significant drop of the *m/z* 202 signal within one hour with the mission current at the correct level indicates a low reagent supply. In this case, you should replace the fluoranthene vial.

Changing the reagent vials requires that the Orbitrap Elite ETD mass spectrometer be placed in Service mode after the vials have cooled. (Vial cooling is done in Off condition.) See the following sections for procedures to be used to change the reagent vials:

- "Placing the Instrument in Off Condition and Service Mode" on page 6-51
- "Installing/Exchanging the Reagent Vials" on page 6-53

NOTICE The ETD reagent vials are designed to keep the ETD reagent out the lab environment. Removal and replacement of the ETD reagent vials when they are not empty causes excessive puncturing of the septums and reduces their integrity. This could result in ETD reagent (fluoranthene) entering the lab environment. To prevent this from occurring, remove and replace the ETD reagent vials only when they are empty. Do not reinstall used vials. ▲

⚠ Store and handle all chemicals in accordance with standard safety procedures. The Material Safety Data Sheet (MSDS) that describe the chemicals being used should be freely available to lab personnel for them to examine at any time. Material Safety Data Sheets (MSDSs) provide summarized information on the hazard and toxicity of specific chemical compounds.

MSDSs also provide information on the proper handling of compounds, first aid for accidental exposure, and procedures for cleaning spills or dealing with leaks. Producers and suppliers of chemical compounds are required by law to provide their customers with the most current health and safety information in the form of an MSDS. Read the MSDS for each chemical you use. Dispose of all laboratory reagents in the appropriate manner (see the MSDS).

[1] Item contained in Inlet Valve Seal Kit.

Safety information about fluoranthene is given in Appendix A, "Fluoranthene."

Placing the Instrument in Off Condition and Service Mode

The power switches control power to the Orbitrap Elite ETD mass spectrometer (MS and ETD Module). The ETD Module power switches control the power to the ETD Module only. When the Orbitrap Elite ETD MS is fully operational (all systems On), the MS Main Power switch is in the On position and the FT Electronics switch is in the operating (On) position.

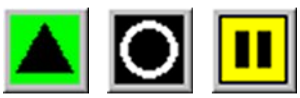
Normally, the ETD Module Power and Service switches remain On. Use the FT Electronics switch on the MS unit to place the Orbitrap Elite ETD mass spectrometer in Service mode. Turn On and Off the instrument (both ETD Module and MS) with the MS Main Power switch.

⚠ CAUTION **Burn Hazard.** When mass spectrometer and ETD Module system are turned On, the flow restrictor, the transfer line heaters, and the ion source heater can be at 160 °C. The vial heaters can be at 108 °C (or set point). Before you replace reagent vials or before you service heated components make sure that they have cooled to a safe temperature for handling.

NOTICE The instructions that follow assume that no analyte is flowing into the API source. ▲

❖ **To place the Orbitrap Elite ETD mass spectrometer in Off Condition and Service mode and to make sure that the vials are safe to handle**

1. If the Tune Plus window is not already open, choose **Start > Programs > Thermo Instruments > LTQ > LTQ Tune** from the taskbar. The Tune Plus window appears. (See Figure 6-10 on page 6-25.)

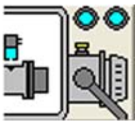


On Off Standby

   You can determine the state of the MS by observing the status of the On/Standby button on the Control/Scan Mode toolbar. The three different statuses of the On/Standby button are shown at the left.

2. Choose **Control > Off** from the Tune Plus pull-down menu to place the system in Off condition. When the mass spectrometer is in Off condition, the Orbitrap Elite ETD MS turns off the ion source sheath gas, auxiliary gas, high voltage, and all of the ETD Module heaters.

   NOTICE Choose **Control > Off** from the Tune Plus pull-down menu to shut down all of the ETD Module heaters. ▲



3. Click the reagent ion source portion of the instrument control icon at the top of the Tune Plus window. The Reagent Ion Source dialog box appears (Figure 6-44).

   Observe the temperature of Vial 1 in the Actual column of the Reagent Ion Source dialog box (Figure 6-44). Nitrogen cooling gas will flow until the vial reaches 70 °C. (See “Turning off the Reagent Ion Source: What to Expect” on page 5-14.) Wait up to 90 minutes for the vial temperature to reach ambient temperature (about 30 °C).

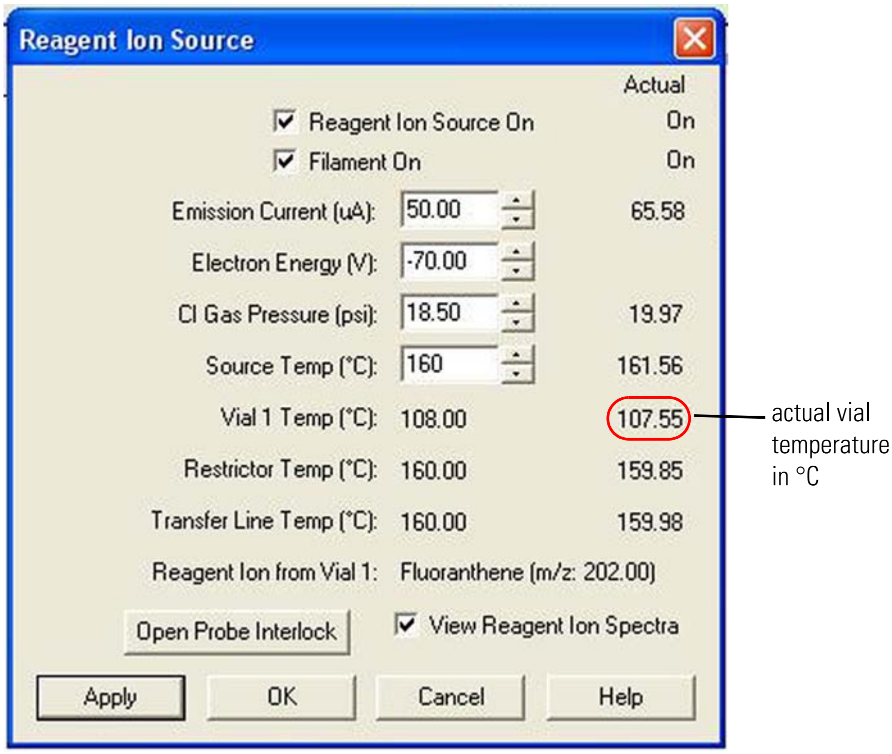


Figure 6-44. Reagent Ion Source dialog box

⚠ CAUTION

Burn Hazard. The vials or the vial holders are still too hot to handle when the cooling nitrogen stops at a vial temperature of 70 °C. Do not touch them immediately after the cooling nitrogen stops. Let the vials cool to about 30 °C (wait for about 90 minutes after the cooling gas stops) before you proceed with the next step and handling the vials.

4. Toggle the FT Electronics switch to Service mode (Off) when the vial has reached a temperature that is safe for handling (about 30 °C). Toggling the FT Electronics switch to Service mode turns off all components except the turbomolecular pumps and the forepumps in both the mass spectrometer and the ETD Module.

NOTICE Do not place the ETD Module Service switch into its Service mode (Off) position while the MS switches are left in their On positions. This could cause communication problems between the MS and the ETD Module. The ability to control the Service mode for both the MS and the ETD Module at one point (at the FT Electronics switch) is a safety feature. ▲

⚠ CAUTION **Burn Hazard.** System temperature monitoring will stop when the system is placed in Service mode. Do not place the system in Service mode until the vials reach a safe temperature (about 30 °C). Do not touch the vials, the vial holders, or the heater assembly until a safe temperature is reached (about 30 °C).

The Orbitrap Elite ETD mass spectrometer is now in Service mode and the vials are at a safe temperature for handling.

Installing/Exchanging the Reagent Vials

After the reagent vial heaters have cooled to room temperature, the reagent vials are ready to be installed or exchanged.

❖ **To install or exchange the reagent vials**

1. Remove the back panel from the ETD Module. (See “Removing the ETD Main Access Panel” on page 6-21.) This exposes the reagent inlet source heating unit, which has its own cover (Figure 6-45 on page 6-54).

⚠ CAUTION **Burn Hazard.** Removing the back panel before the system is placed in Service mode will open the panel electrical interlocks and stop all system activity including temperature monitoring. In the absence of temperature monitoring, you might try to handle the vials before it is safe to do so. Follow the procedures described in “Placing the Instrument in Off Condition and Service Mode” on page 6-51 before you remove the back panel of the ETD Module.

2. Make sure that the vial heater cover is cool to the touch.

⚠ CAUTION **Burn Hazard.** The vial heaters can be at 108 °C (or set point). Let the vials cool for a sufficient time (up to 90 minutes) and then place the system in Service mode. (See “Placing the Instrument in Off Condition and Service Mode” on page 6-51.) Make sure that the vial heater cover is safe to handle before you remove the vial holders and the reagent vials.

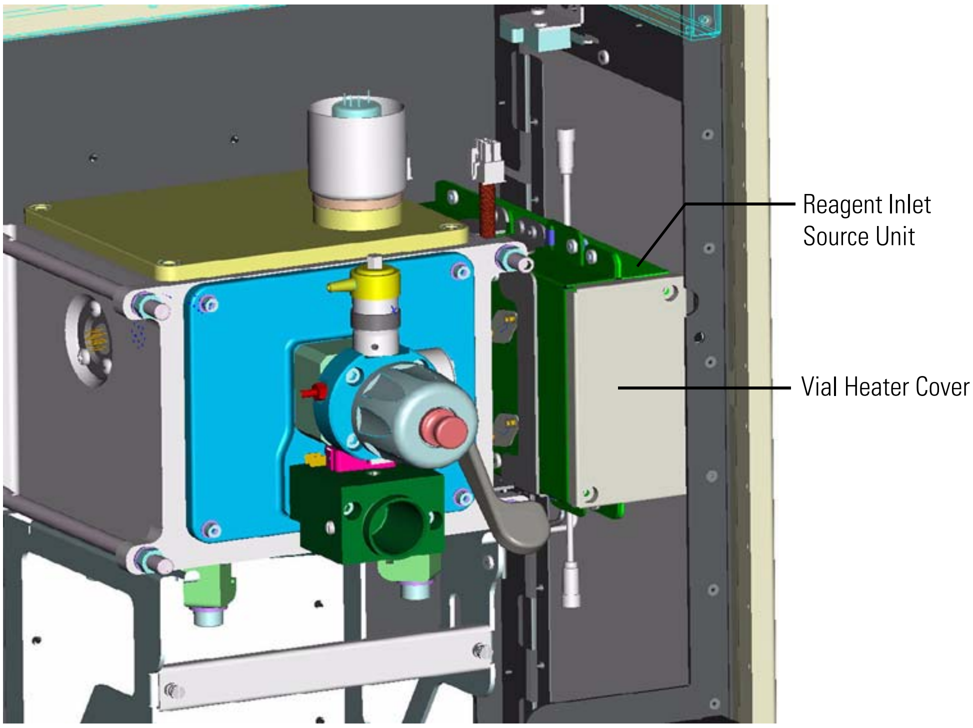


Figure 6-45. ETD Module with back panel removed

3. Put on a pair of new, white nitrile clean room gloves and protective eye wear.

4. With a Phillips screwdriver, remove the screws in the vial heater cover. The vial heater cover is on the right side of the ETD Module as you view it from the back of the Orbitrap Elite ETD mass spectrometer (Figure 6-45).

5. Remove the vial holder by gently pulling it out of the vial heater.

6. Remove the empty vial if it is present. The vial holder is a cylindrical tube with a handling knob at one end and ribs along its length. See Figure 6-46. These ribs prevent the vial holder from rotating when it is placed into the vial heater. Figure 6-47 on page 6-55 shows the tab and ribs of a vial holder in the vial heater.

   NOTICE Dispose of an empty fluoranthene vial in accordance with its MSDS. ▲

⚠ 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.

Figure 6-46. Reagent vials with holders

7. Take a vial that contains the ETD reagent (fluoranthene) from its box and remove the aluminum tab from the top of the vial's crimp seal.
8. Put the vial into a vial holder.

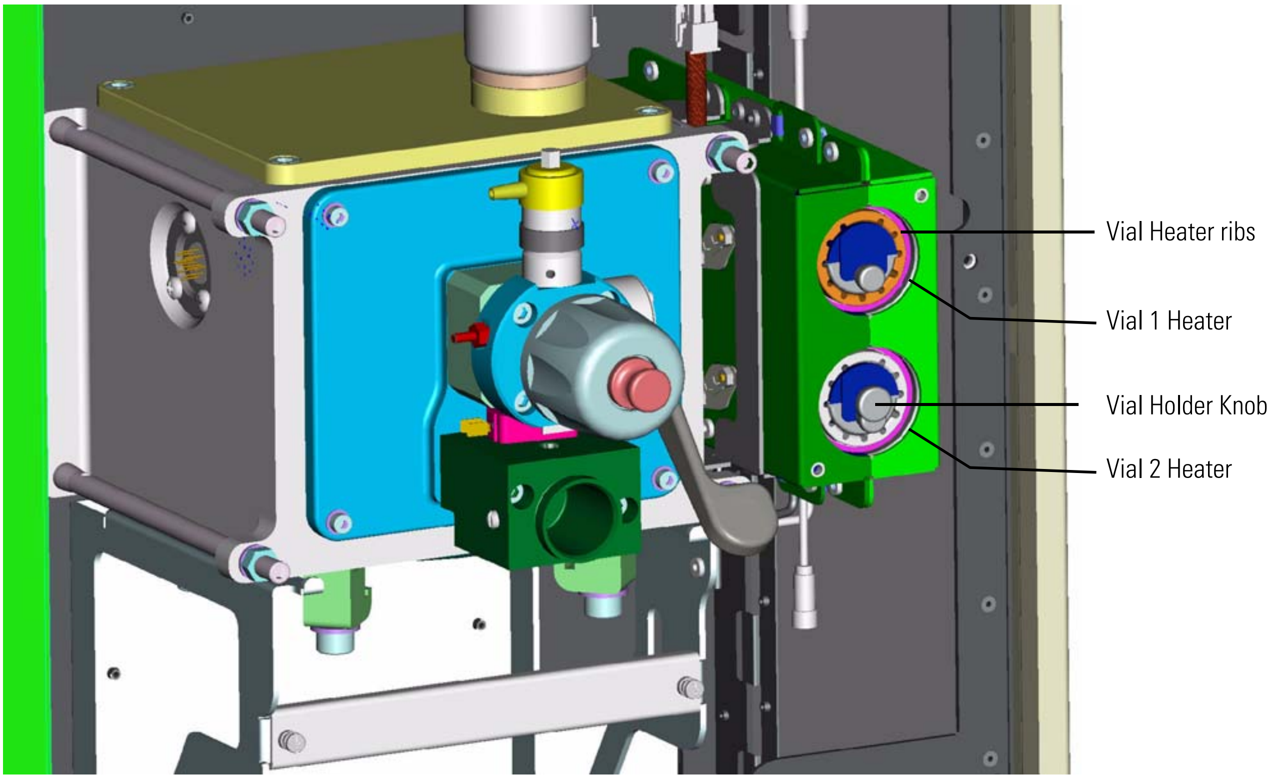


Figure 6-47. ETD Module with vial heater cover removed

9. Put this ETD reagent vial and its vial holder into the Vial 1 heater (top vial heater). Gently slide the vial holder into the vial heater.

10. Put the empty vial from the box into the other vial holder if an empty vial is not already installed.

11. Put this empty vial and its vial holder into the Vial 2 heater (bottom vial heater) if an empty vial is not already installed.

⚠ CAUTION

Hazardous Chemicals. Health Hazard. The empty vial in the Vial 2 heater is an integral part of the carrier/CI gas system. It is necessary to keep the carrier/CI gas system closed to the laboratory. If no vial is placed in the Vial 2 heater, the carrier/CI gas that contains the reagent might escape to the laboratory and cause a safety problem.

NOTICE If no vial is placed in the Vial 2 heater, the ETD Module will not operate correctly and the filament will burn out. ▲

12. Reinstall the vial heater cover over the vial heaters.

13. Reinstall the back panel of the ETD Module. See "Removing the ETD Main Access Panel" on page 6-21. The ETD Module will not turn on unless the back panel is installed.

14. Start the system:

    a. Toggle the FT Electronics switch to the On position.
    The system will boot to Standby mode. Then ion source heater, the flow restrictor, and the transfer line heaters will start heating. Monitor these temperatures in the Status View on the right side of the Tune Plus window. (See Figure 6-10 on page 6-25.) They will have green check marks when they have reached their operating temperatures.

    b. Select the Reagent Ion Source On check box in the Reagent Ion Source dialog box when the ion source heater, the flow restrictor, and the transfer line heaters are at their operating temperatures. (See Figure 6-44 on page 6-52.)

The Orbitrap Elite ETD mass spectrometer is now ready for use.

Changing the Reagent Ion Source Flow Restrictors

❖ **To change the reagent ion source flow restrictors**

1. Shut down completely the instrument according to the procedures in "Shutting Down the Orbitrap Elite Mass Spectrometer Completely" on page 5-7.

⚠ CAUTION **Burn Hazard.** The reagent vial heaters can be 108 °C (or set point), the flow restrictor, the transfer line heaters, and the ion source heater can be at 160 °C. These components might be too hot to touch. Make sure that all of these components are safe to touch before you handle them.

2. Remove the ETD side access panel according to the instructions in "Removing the ETD Side Access Panel" on page 6-22.

   NOTICE The ETD side access panel is interlocked with the ETD Module power. When the ETD side access panel is removed, all power to the ETD Module will be turned off. ▲

3. Remove the four screws that hold the reagent inlet cover in place.

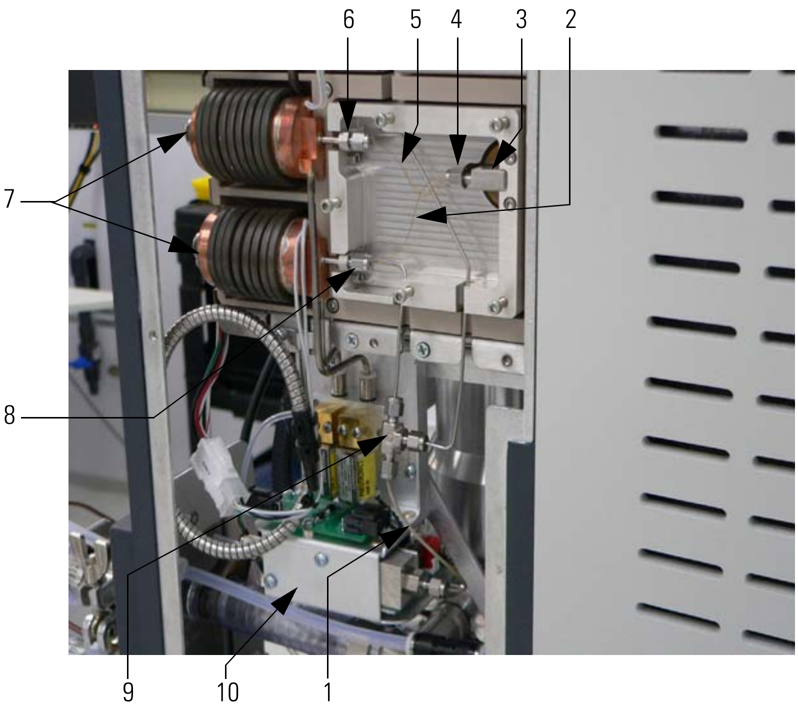
⚠ CAUTION **Burn Hazard.** The reagent inlet cover might be too hot to touch. Make sure that the reagent inlet cover is at or near room temperature before you handle it.

4. Remove the five screws that hold the restrictor oven cover in place.

⚠ CAUTION **Burn Hazard.** The restrictor oven cover might be too hot to touch. Make sure that the restrictor oven cover is at or near room temperature before you handle it.

5. Replace both fused silica restrictors and their ferrules by removing their Swagelok™ nuts. See Figure 6-48 on page 6-58.
6. Thread two pieces of fused silica tubing into the two hole ferrule from the Installation Kit for the Reagent Inlet Module. Place a Swagelok fitting over the ferrule.
7. Insert the two hole ferrule and Swagelok fitting from step 6 onto the transfer line inlet (item 3 in Figure 6-48) and tighten the Swagelok fitting.
8. Thread the opposite end of one of the pieces of fused silica tubing into a single hole ferrule. Place a Swagelok fitting over the ferrule.
9. Insert the ferrule and Swagelok fitting from step 8 on to one of the oven outlets (items 6 or 8 in Figure 6-48) and tighten the Swagelok fitting.

   NOTICE Do not overtighten the ferrules. The ferrules might loosen after they are first heated. If this occurs, then retighten them. ▲



Labeled components: 1=PEEKsil™ tubing, 2=fused silica tubing from lower oven, 3=transfer line inlet, 4=Swagelok fitting with two hole ferrule, 5=fused silica tubing from upper oven, 6=upper oven Swagelok fitting with a single hole ferrule, 7=vial 1 (upper) and vial 2 (lower) heaters, 8=lower oven Swagelok fitting with a single hole ferrule, 9=Tee below reagent inlet assembly, 10=gas valves

Figure 6-48. Reagent inlet assembly

10. Repeat step 9 for the other oven.

11. Replace the restrictor oven cover and reagent inlet cover removed in step 3 and step 4.

12. Loosen the Swagelok fitting connecting the PEEKsil™ tubing (item 1 in Figure 6-48) to the Tee below the reagent inlet assembly (item 9 in Figure 6-48) and from the gas valves (item 10 in Figure 6-48).

13. Replace the old PEEKsil tubing with new PEEKsil tubing from the Installation Kit for the Reagent Inlet Module.

14. Close the ETD Module and restart the instrument. Follow the procedures given in "Starting up the System after a Shutdown" on page 5-9.

Cleaning the Fan Filters of the ETD Module

Clean the fan filters every four months. The fan filters are at the rear of the ETD Module on the left side (as viewed from the back of the ETD Module). See Figure 6-49.

Figure 6-49. ETD Module, top panel

❖ **To clean the fan filters of the ETD Module**

1. Remove the fan filter from the rear of the ETD Module by pulling it out of the fan filter bracket.
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 let them to air dry.
5. Reinstall the fan filter in the fan filter bracket.

Maintenance of the Cooling Circuit

The recirculating chiller and the water filter require maintenance on a regular basis.

Maintenance for the Recirculating Chiller

For the Thermo Scientific ThermoFlex™ 900 recirculating chiller, the checks described in this section should be carried out on a regular basis.

NOTICE For further information and maintenance instructions, refer to the manufacturer's manual supplied with the instrument. ▲

Reservoir

Periodically inspect the fluid inside the reservoir. If cleaning is necessary, flush the reservoir with a cleaning fluid compatible with the circulating system and the cooling fluid.

The cooling fluid should be replaced periodically. The replacement frequency depends on the operating environment and the amount of usage.

⚠ CAUTION **High Temperatures.** Burn Hazard. Before you change the operating fluid, make sure that it is at safe handling temperature.

Fluid Bag Filter

The ThermoFlex 900 recirculating chiller that is installed in the cooling circuit of the instrument is equipped with a fluid bag filter, which needs to be replaced on a regular basis. Replacement bags are available from Thermo Fisher Scientific.

Condenser Filter

To prevent a loss of cooling capacity and a premature failure of the cooling system, clean the condenser filter regularly. If necessary, replace it.

Replacing the Water Filter Cartridge

The filter removes particulate matter in the cooling system that might cause damage to the flow sensor. The filter cartridge should be replaced annually or as necessary. A replacement is available from Thermo Fisher Scientific.

❖ **To replace the water filter cartridge**

1. Place the system in Standby condition as described on page 5-4.

2. Switch off the chiller.

3. The filter is installed on the left instrument side, in the cooling lines of the Orbitrap system between the Peltier element and the flow sensor. See Figure 6-50. Quick couplings connect the filter assembly to the hoses of the cooling lines. Press the thumb latch of each quick coupling to release it. Valves in the couplings prevent the water from leaking out. Then remove the complete filter assembly.

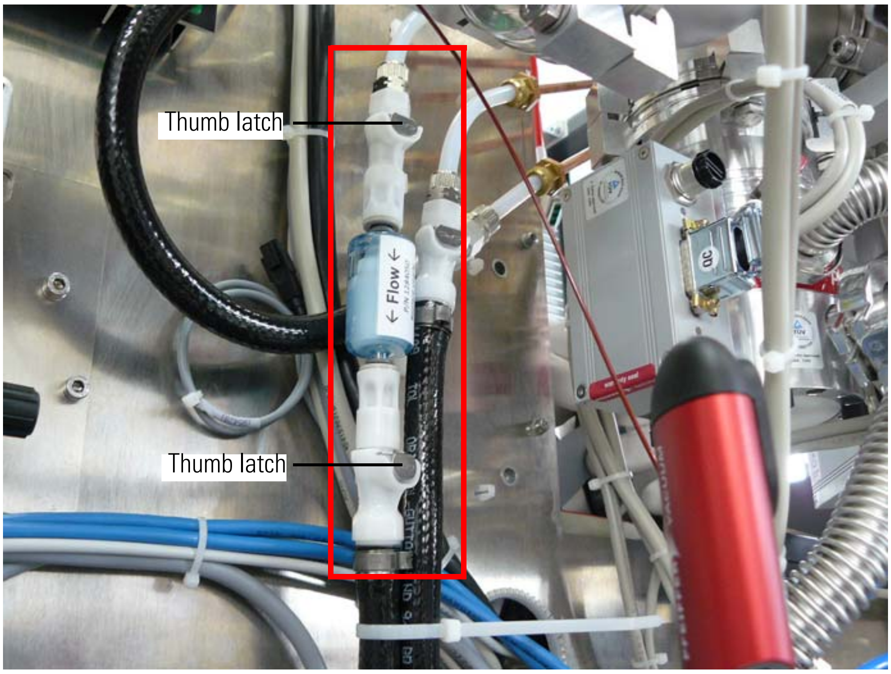


Figure 6-50. Installed water filter

4. Remove the filter from the assembly by using a 5/16 inch wrench and pressing against the gray ring on the quick coupling, away from the filter. See Figure 6-51.

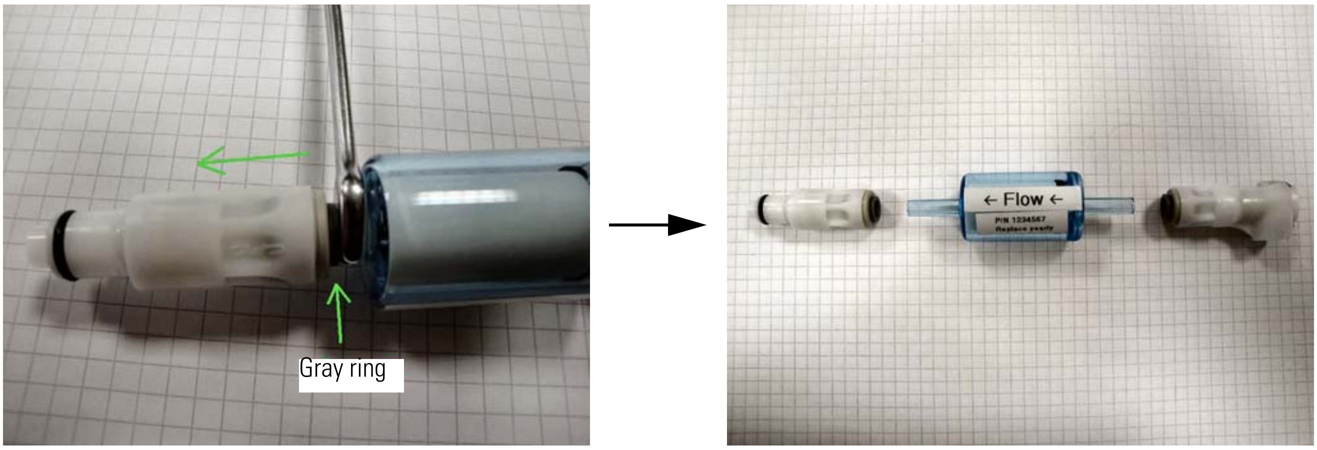


Figure 6-51. Removing the filter cartridge

5. Insert the new filter into the quick couplings. See Figure 6-52.

Figure 6-52. Filter cartridge with Quick couplers

> **NOTICE** Pay special attention to the direction of flow. Reversing the flow can damage both the flow sensor and the filter. ▲

6. Connect the filter assembly to the hoses of the cooling lines.
7. Switch on the chiller system. Check for leaks and check the water level in the chiller. Refill as appropriate.
8. Set the instrument to operating condition.

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

⚠ 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 for exchange or repair.

If hazardous materials have contaminated instrument parts, then 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 present materials 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 you are unsure whether parts of the system are possibly contaminated by hazardous material, then make sure that the Thermo Fisher Scientific field service engineer is informed before the engineer starts working on the system.

Returning Parts

To protect our employees, we ask you for some special precautions when you send parts back to the factory for exchange or repair.

Your signature on the Health and Safety Form confirms that the returned parts have been decontaminated and that they are free of hazardous materials. This form is available on page B-7. Instead of copying or printing this page, request a copy from the Thermo Fisher Scientific field service engineer.

Chapter 7 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 Orbitrap Elite system, order only the parts listed or their equivalent.

NOTICE Not all parts are available for purchase separately. Some parts may only be available for purchase as part of a kit or assembly. ▲

For information on how to order parts, see "Contacting Us" on page 1-5.

Contents

Ion Sources

ESI probe, for Ion Max source	OPTON-20011
Low flow metal needle for API 2 probes	OPTON-30004
Nanospray II Ion Source	OPTON-20050
Static Nanospray	OPTON-20051
Dynamic Nanospray	OPTON-97017
APCI probe	OPTON-20012
APPI probe	OPTON-20026
HESI-II Probe Kit	OPTON 20037
High-flow needle insert assembly	OPTON-53010
Low-flow needle insert assembly	OPTON-53011

Parts for the Basic System

Orbitrap Analyzer Installation Kit

Tube, 1/8” × 2.1- 1.4301 0261000
Ferrule, stainless steel; R. 1/8” 0520950
Ferrule, stainless steel; V. 1/8” 0522520
Cap nut, stainless steel; 1/8“. 0520890
Fitting KJH06-00. 1221620

Pumping System

For a schematical overview of the pumping system, see Figure 2-22 on page 2-30.

T-piece 13 mm. 0512360
Hose 13 × 3.5; PVC. 0690720
Turbomolecular pump HiPace 300. 1272910
Turbomolecular pump; HiPace 80 1272920
UHV gauge IKR 270; short 1181380
Compact Pirani Gauge TPR280. 1156400
Water cooling for HiPace 300. 1272930
Water cooling for HiPace 80. 0794742
PVC hose, with steel helix; ID=45 mm, L=1.6 m. 1184330
Hose nipple, DN 40, ISO-KF-45. 1159230
Venting flange; DN 10, KF-G1/8”. 1184400
Splinter shield for TMPs, with DN 100 CF-F flange 1198590
Centering ring, with integrated splinter shield; DN 63 ISO. 1198600
Anti-magnetic cover for IKR 270 1181390
Gasket; NW 100 CF, copper 0552440
Hose, metal; KF16-KF25 - 250mm 1154130
Gasket; copper, NW 35 0550480
Metal tube, KF NW16×250. 0524260
KF Tee piece; NW 16 KF, stainless steel 0524230
Centering ring with o-ring; DN 16, Viton .0522140
Centering ring with o-ring; DN 25, Viton .0522150
Centering ring; NW 16/10, aluminum-Viton 0522200
Clamping ring; NW 10/16, KF 0521830
Clamping ring; NW 20/25, KF 0521560
Reducing cross piece; DN40/DN16 KF. 1184310
Metal tube; DN40x500 1184350
Metal tube; DN40x750 1181290
Hose clamp; NW 40 1181320
Centering ring; NW 40 KF, aluminum-Viton 0522260
Tension ring; NW 32/40 KF 1181250
Clamping screw; DN63-100 ISO, aluminum. 1042670
Flexible metal hose KF NW 16x500. 0534500
Lubricant reservoir HiPace 80 1275740
Lubricant reservoir HiPace 300 1275730

Water Supply

For a schematical overview of the cooling water circuit, see Figure 2-30 on page 2-41.

Quick coupling insert; 9.6 mm 1141640
Quick coupling body; 9.6 mm. 1138960
Hose; 9 x 3, black, PVC 1049540
Hose; 6 x 1, Teflon 1042660
Quick coupling insert; Delrin Acetal, NW 6.4 1185030
Quick coupling body; Delrin Acetal, NW 6.4 1185020
Clamping piece 8/16 0370130
Adaptor hose nipple; male, 1/2 x 10 1185840
Flow control sensor 1191740
Filter cartridge; 50 µm DIF 1284050

Gas Supply

For a schematical overview of the gas supply, see Figure 2-27 on page 2-37.

Bulkhead union; 1/16”, for hose 4 x 1 (for P/N 069 1130) 1153660
Bulkhead union; 1/8”×1/8” 0523450
Hose; 4 x 1, Teflon 0690280
Hose; 4 x 1, polyurethane, blue 0691130
Capillary 1/16” ID-SS 0605470
Plug-in T-piece; 3 x 6mm 1128140
Regulator + manometer f. Orbitrap analyzer 1257670
Capillary; 1/16”x0.13x400mm (red), PEEK 1253830
Coupling; 1/16”, SS-100-6 0524340
Ferrule; 1/16” GVF 16-000. 1121110
Reducer Swagelok; 1/8” × 1/16”, stainless steel 0662880
Ferrule; 1/16” GVF/16 0674800
Connector 1/8”, for hose OD 4 mm 1128680
Cap nut; 1/16”, stainless steel 0520880
Hose; 2 x 1, PTFE. 1091650
Sleeve; Ø 6 mm 1047320
Capillary; PEEKsil, 1/16”, 0.1 × 500 mm 1223420
Plug, KQ2P-06 1185620
Cap, KQ2C-06 1258220
Swagelok™-type nut, brass, 1/8 in. ID 00101-15500
Ferrule, two-piece set, brass, back, 1/8 in. ID 00101-02500
Ferrule, two-piece set, brass, front, 1/8 in. ID 00101-08500

Parts Lists for the ETD System

This section contains parts lists for the components of the ETD System of the Orbitrap Elite ETD mass spectrometer.

Quadrupole Orbitrap analyzer, complete 1239200
Housing HCD/ETD 1231740
Separating plate HCD/ETD 1231770
Screw M 4 x 8 DIN912 1044420
O-ring 129 X 4 A Viton. 1240520
Lid HCD/ETD 1231760
Screw-in connector; 1/16” 1186150
Gasket; NW 63 ISO, aluminum/Viton 0554060
Blank flange; stainless steel, NW 63 0652620
Clamping screw; DN63-100, aluminum 1028380
Washer 8.4; stainless steel 0470070
Screw, hexagonal; M 8 x 35, stainless steel 0454400
Washer 8.4 x 11 x 1.5, stainless steel. 0470860
Screw M8 x 35; stainless steel 0454250
Centering ring NW 16 Viton. 0522140
Feedthrough; 8-fold 1,5kV DN16KF. 1231750
O-ring; 118 X 5 A, Viton. 1168240
Box f. feedthrough; KF16 / Sub-D9 1231800
Cylindrical Screw ISO4762-M6X12-A4. 0453300
Filament Assembly DSQ II 120320-0030
Aluminum oxide abrasive, number 600 32000-60340

Vacuum System ETD

Flange clamp; KF16 1145860
PUMP, TURBO, EDWARDS EXT75DX ISO100, TNR . . 00108-01-00016
Splinter guard, DN_63_ISO 1198600
Metal hose, DN 16 ISO-KF x500 1181410
Centering ring with o-ring; DN 16, Viton .0522140
Clamping ring; NW 10/16, KF 0521830
Hose flange; NW 25 KF. 1042330
Centering ring, with o ring; DN 25, Viton. 0522150
Clamping ring, DN 25. 0521560
Flange, KF16 - hose OD 19 1239340
Reducer; DN 16/DN 25, aluminum 0522160
PUMP, ROTARY VANE, EDWARDS RV3. 00108-01-0008
KIT, ACCESSORY, MECHANICAL PUMP, RV3 98000-620007
Forepump oil, 1 L 00301-15101

Gas Supply ETD

Plug-in T-piece; 3 x 6mm 1128140
Sleeve 6 mm 1047320
Reducing hose connector, 3.2—>6. 1239220

Hose cutter 1239280
T-piece 13 mm 0512360
Hose 9 X 3; PVC, black. 1049540
Clamping piece 8/16 0370130
Hose; 4 X 1, Teflon 0690280
Clamping ring; stainless steel, NW10/16. 1149200
PEEK capillary; 1/16” x 0.040. 1245940
Ferrule, 1/16”, for GVF/16 0674800
Ferrule 1/16” - CTFE, collapsible 1224700

Electronic Parts ETD

Cable Y-ADAPTER/T.PUMP 2108630
Coupling; RJ45 BU/2BU 2075210
Patch cable; 0.51MT RJ45 gray SFTP. 2080870
Cable POWER DIS./T-PUMP 2081200
Cable CLT-OFFSET-A 2108710
Cable IOS ETD/ION OPTIC-S. 2108820
UNIT_ION OPTIC SUPPLY ETD 2108920
PCB LTQ CABLE DRIVER. 2097780
PCB ORBITRAP CABLE RECEIVER. 2097830
PCB ETD CABLE RECEIVER 2097800
Cable ETD/LTQ/ORBITRAP-INTERCONNECT 60 2108940
Cable ETD/LTQ/ORBITRAP-INTERCONNECT 36 2108950
Cable ETD/LTQ/ORBITRAP-INTERCON SUPPLY 2108960
Coaxial cable; ETD IOS/ANALOG CTRL, J5554 2108990
Coaxial cable; ETD IOS/ANALOG CTRL, J5555 2109000
Coaxial cable; ETD IOS/ANALOG CTRL, J5556 2109010
Cable ANALOG CTRL / ETD IOS 2108970
Cable ETD IOS/HCD multipole 2108980
Extension cable; 16A C20-C19 2M 2097050
ADAPTER_IOS/MULTIPOLE-HCD 2100410

Reagent Inlet Module

Ion volume insertion and removal tool 98000-60028

Inlet Valve Seal Kit 119265-0003
Inlet valve seal removal tool. 119283-0001
Spool inlet valve seal 119683-0100
O-ring, Viton, 0.530 in. ID × 0.082 in. *w* 3814-6530

Reagent Inlet Module Installation Kit

Reagent Inlet Module Installation Kit 98000-62006
Ferrule, back, PTFE, for Swagelok 1/16 in. tube. 00101-08-00008
Ferrule, front, PTFE, for Swagelok 1/16 in. tube 00101-08-00007
Ferrule, Vespel/graphite, 1-hole, 1/16 in. OD,
0.4 mm ID 00101-08-00005

Ferrule, Vespel/graphite, 2-holes, 1/16 in. OD,
0.4 mm ID 00101-08-00006
Tubing, fused silica, 0.363 in. OD, 0.1 mm ID,
100 mm long 98000-20060
Tubing, PEEKsil™, 1/16 in. OD, 0.05 mm ID,
100 mm long 00109-02-00021

ETD Reagent Kit

ETD Reagent Kit 98000-62008
Angiotensin I, 1 mg 00301-15517
Fluoranthene, 150 mg 00301-01-0013

The fluoranthene in your ETD Reagent Kit is Sigma/Aldrich Supelco #48535. The fluoranthene MSDS is obtained from the MSDS link at:

www.sigmaaldrich.com/catalog/search/ProductDetail/SUPELCO/48535

Thermo Fisher Scientific supplies fluoranthene as a two vial kit. One vial contains 150 mg of fluoranthene and the other is the required empty vial.

The angiotensin I in your ETD Reagent Kit is Angiotensin I human acetate hydrate (Sigma/Aldrich #A9650). Angiotensin I is potentially hazardous. Handle it in accordance with its MSDS. The angiotensin I MSDS is obtained from the MSDS link at:

www.sigmaaldrich.com/catalog/search/ProductDetail/SIGMA/A9650

Appendix A Fluoranthene

Fluoranthene is used as the Electron Transfer Dissociation (ETD) reagent in the ETD Module portion of the Orbitrap Elite ETD mass spectrometer. The fluoranthene radical anion is generated according to the reaction shown in Figure A-1.

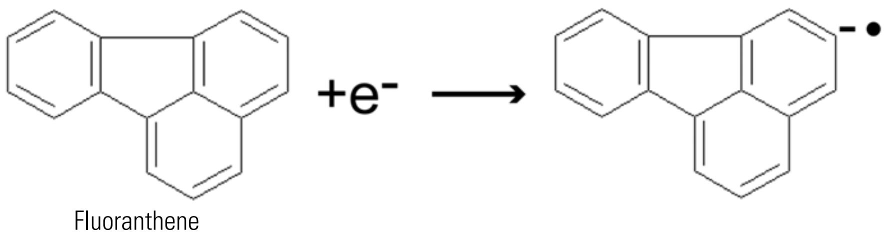


Figure A-1. ETD Reagent (fluoranthene radical anion) generation from fluoranthene

Fluoranthene is potentially hazardous. Use it in accordance with its Material Safety Data Sheet (MSDS).

Store and handle all chemicals in accordance with standard safety procedures. The Material Safety Data Sheet (MSDS) describing the chemicals being used should be freely available to lab personnel for them to examine at any time. Material Safety Data Sheets (MSDSs) provide summarized information on the hazard and toxicity of specific chemical compounds.

MSDSs also provide information on the proper handling of compounds, first aid for accidental exposure, and procedures for cleaning spills or dealing with leaks. Producers and suppliers of chemical compounds are required by law to provide their customers with the most current health and safety information in the form of an MSDS. Read the MSDS for each chemical you use. Dispose of all laboratory reagents in the appropriate manner (see the MSDS).

The fluoranthene contained in the ETD Reagent Kit (see page 7-7) is Sigma/Aldrich Supelco #48535. The fluoranthene MSDS is obtained from the MSDS link at:

www.sigmaaldrich.com/catalog/search/ProductDetail/SUPELCO/48535

Thermo Fisher Scientific supplies fluoranthene as a two vial kit. One vial contains 150 mg of fluoranthene and the other is the required empty vial.

Fluoranthene

Appendix B Legal Documents

Contents

FCC Compliance Statement

THIS DEVICE COMPLIES WITH PART 18 OF THE FCC RULES.

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 (Orbitrap Elite)

-Original-

EG-Konformitätserklärung
EC Declaration of Conformity

CE

ThermoFisher
SCIENTIFIC

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

Wir erklären hiermit, dass die folgenden Produkte
We hereby declare that the following products

Bezeichnung: *Designation:*	**Massenspektrometer** *Mass Spectrometer*
Modell: *Model:*	**Thermo Scientific Orbitrap Elite** *Thermo Scientific Orbitrap Elite*

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

Maschinenrichtlinie *Machinery Directive*	**2006/42/EG** *2006/42/EC*
Richtlinie über elektromagnetische Verträglichkeit *Electromagnetic Compatibility Directive*	**2014/30/EU** *2014/30/EU*
RoHS-Richtlinie *RoHS Directive*	**2011/65/EU** *2011/65/EU*

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

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

ppa. Jörg Behrens

Unterschrift
Signature

Bremen, 2017-05-17

Datum
Date

Declaration of Conformity (Velos Pro / Velos Pro ETD)

Regulatory Compliance

Thermo Fisher Scientific performs complete testing and evaluation of its products to ensure full compliance with applicable domestic and international regulations. When the system is delivered to you, it meets all pertinent electromagnetic compatibility (EMC) and safety standards as described in the next section or sections by product name.

Changes that you make to your system may void compliance with one or more of these EMC and safety standards. Changes to your system include replacing a part or adding components, options, or peripherals not specifically authorized and qualified by Thermo Fisher Scientific. To ensure continued compliance with EMC and safety standards, replacement parts and additional components, options, and peripherals must be ordered from Thermo Fisher Scientific or one of its authorized representatives.

Velos Pro Mass Spectrometer (April 2011)

EMC Directive 2004/108/EEC

EMC compliance has been evaluated by TÜV Rheinland of North America, Inc.

EN 61326-1: 2006
EN 55011: 2007, A2: 2007
CFR 47, FCC Part 15, Subpart B, Class A: 2009
EN 61000-3-2: 2006
EN 61000-3-3: 1995, A1: 2001, A2: 2005
EN 61000-4-2: 1995, A1: 1999, A2: 2001
EN 61000-4-3: 2006
EN 61000-4-4: 2004
EN 61000-4-5: 2005
EN 61000-4-6: 2007
EN 61000-4-11: 2004

Low Voltage Safety Compliance

This device complies with Low Voltage Directive 2006/95/EEC and harmonized standard EN 61010-1:2001.

Velos Pro/ETD System (April 2011)

EMC Directive 2004/108/EEC

EMC compliance has been evaluated by TÜV Rheinland of North America, Inc.

EN 61326-1: 2006
EN 55011: 2007, A2: 2007
CFR 47, FCC Part 15, Subpart B, Class A: 2009
EN 61000-4-3: 2006
EN 61000-4-4: 2004
EN 61000-4-5: 2005

EN 61000-3-2: 2006
EN 61000-3-3: 1995, A1: 2001, A2: 2005
EN 61000-4-2: 1995, A1: 1999, A2: 2001
EN 61000-4-6: 2007
EN 61000-4-8: 1993, A1: 2001
EN 61000-4-11: 2004

Low Voltage Safety Compliance

This device complies with Low Voltage Directive 2006/95/EEC and harmonized standard EN 61010-1:2001.

Health and Safety Form

This Decontamination Declaration Form must be completed for all materials returned to Thermo Fisher Scientific, it should be sent to the destination by e-mail after printing and with an authorization signature. A hard copy should be attached to the outside of the package with shipping paperwork and a further copy should be placed inside the packaging. The receiving Thermo Fisher Scientific office can help with this form and supply a return number, shipping address and e-mail address. Use the text "not used" to indicate a field not being used. Where a Thermo Scientific part number is not known, add the supplier name (as for the examples below).

---

1. General Information

Customer	______________________	Instrument type	______________
Address	______________________	Instrument SN	______________
	______________________	Order number	______________
Phone	______________________	Return number	______________
E-Mail	______________________		

Part Number	Quantity	Material Description	Error Description / Reason for Return	Return Part Serial #
e.g. Thermo Scientific PN				
e.g. Pfeiffer				
e.g. Leybold				
e.g. Edwards				

---

2. Condition of the material or instrument

Has the material or instrumentation been removed from the shipping packaging or in contact with

- pump fluids,
- service fluids,
- samples,
- standard solutions,
- other chemicals,
- or hazardous materials?

Tick the applicable check box.

☐ Yes → go to section 3

☐ No → go to section 5

---

3. Contamination

To which compounds has the material/instrumentation been exposed? Biological or radioactive contaminated materials must not be shipped to Thermo Fisher Scientific. If any of the check boxes are ticked, go to section 4. If 'No ticks' is ticked, go to section 5.

☐ toxic	☐ flammable	☐ serious health hazard
☐ corrosive	☐ oxidizing	☐ hazardous to environment
☐ explosive	☐ gas under pressure	☐ other harmful substances

Tick the applicable check box.

☐ At least one tick → go to section 4

☐ No ticks → go to section 5

ThermoFisher SCIENTIFIC

Health and Safety Form

4. Description of Process Substances and/or Compound

Which substances have been in contact with the material or instrumentation? (trade name and/or chemical term of service fluids and substances; properties of substances or compounds according to material safety data sheet; e.g. toxic, flammable, corrosive, radioactive)

	Part Number	Serial Number	Trade Name	Chemical / Substance Name / Properties
a)				
b)				
c)				
d)				
e)				
f)				

5. Legally binding declaration

Has the material/instrument undergone a decontamination process?	☐ Yes → go to section 6	☐ No
Is the material/instrument safe to handle for Thermo Fisher Scientific and third party personnel?	☐ Yes	☐ No

Components, materials and/or instruments that have been contaminated to a harmful level by whatever substances and/or compounds as stated in sections 3. and 4. above will not be accepted without written evidence of proper decontamination.
I hereby declare that the instrument has undergone successfully all required decontamination procedures and is safe to handle for Thermo Fisher Scientific and/or third party service personnel or suppliers such as Pfeiffer Vacuum, Leybold Vacuum, Edwards Vacuum products, or others.
I confirm that all information, which is supplied on this form, is accurate, complete and sufficient to judge any contamination level. I acknowledge and agree that I will be liable for any personal injury or any other damage, which might result from a false, inaccurate or incomplete statement and that I will indemnify and defend Thermo Fisher Scientific and/or any other concerned third party for and against any liabilities, claims, losses, and/or damages of all kinds arising out of and/or caused by such false, inaccurate or incomplete statements.
Thermo Fisher Scientific reserves the right not to process refunds or returns where the declared or observed use or previous contamination of the product/material has by Thermo Fisher Scientific judgement impacted its integrity.

6. Detailed description of the Decontamination Process used

Part Number	Serial Number	Describe the decontamination process

Return Number	Name of authorized person (block letters)	Date	Signature	Company stamp

Glossary

This section lists and defines terms used in this guide. It also includes acronyms, metric prefixes, symbols, and abbreviations.

A B C D E F G H I J K L M N O P Q R S T U V W X Y Z

A

A ampere

AC alternating current

ADC analog-to-digital converter; a device that converts data from analog to digital form.

adduct ion An ion formed by the joining together of two species, usually an ion and a molecule, and often within the ion source, to form an ion containing all the constituent atoms of both species.

AGC™ See Automatic Gain Control™ (AGC).

APCI See atmospheric pressure chemical ionization (APCI).

APCI corona discharge current The ion current carried by the charged particles in the APCI source. The voltage on the APCI corona discharge needle supplies the potential required to ionize the particles. The APCI corona discharge current is set; the APCI corona discharge voltage varies, as required, to maintain the set discharge current.

See also corona discharge and APCI corona discharge voltage.

APCI corona discharge voltage The high voltage that is applied to the corona discharge needle in the APCI source to produce the APCI corona discharge. The corona discharge voltage varies, as required, to maintain the set APCI spray current.

See also APCI spray current.

APCI manifold The manifold that houses the APCI sample tube and nozzle, and contains the plumbing for the sheath and auxiliary gas.

APCI needle, corona discharge A needle to which a sufficiently high voltage (typically ±3 to ±5 kV) is applied to produce a chemical ionization plasma by the corona discharge mechanism.

See also chemical ionization (CI), chemical ionization (CI) plasma, atmospheric pressure chemical ionization (APCI), and corona discharge.

APCI nozzle The nozzle in the APCI probe that sprays the sample solution into a fine mist.

See also atmospheric pressure chemical ionization (APCI).

APCI sample tube A fused silica tube that delivers sample solution to the APCI nozzle. The APCI sample tube extends from the sample inlet to the APCI nozzle.

See also atmospheric pressure chemical ionization (APCI), and API stack.

APCI source Contains the APCI probe assembly, APCI manifold, and API stack.

See also atmospheric pressure chemical ionization (APCI), APCI manifold, and API stack.

APCI spray current The ion current carried by the charged particles in the APCI source. The APCI corona discharge voltage varies, as required, to maintain the set spray current.

APCI vaporizer A heated tube that vaporizes the sample solution as the solution exits the sample tube and enters the atmospheric pressure region of the APCI source.

See also atmospheric pressure chemical ionization (APCI).

API See atmospheric pressure ionization (API).

API atmospheric pressure region The first of two chambers in the API source. Also referred to as the spray chamber.

API capillary-skimmer region The area between the capillary and the skimmer, which is surrounded by the tube lens. It is also the area of first-stage evacuation in the API source.

API heated capillary A tube assembly that assists in desolvating ions that are produced by the ESI or APCI probe.

See also API heated capillary voltage.

API heated capillary voltage The DC voltage applied to the heated capillary. The voltage is positive for positive ions and negative for negative ions.

See also API source and API heated capillary.

API ion transfer capillary A tube assembly that assists in desolvating ions that are produced by the ESI, NSI, or APCI probe.

See also API ion transfer capillary offset voltage and API ion transfer capillary temperature.

API ion transfer capillary offset voltage A DC voltage applied to the ion transfer capillary. The voltage is positive for positive ions and negative for negative ions.

See also API source and API ion transfer capillary.

API ion transfer capillary temperature The temperature of the ion transfer capillary, which should be adjusted for different flow rates.

See also API source and API ion transfer capillary.

API source The sample interface between the LC and the mass spectrometer. It consists of the API probe (ESI or APCI) and API stack.

See also atmospheric pressure ionization (API), ESI source, APCI source, ESI probe, and API stack.

API spray chamber The first of two chambers in the API source. In this chamber the sample liquid exits the probe and is sprayed into a fine mist (ESI or NSI) or is vaporized (APCI) as it is transported to the entrance end of the ion transfer capillary.

API spray shield A stainless steel, cylindrical vessel that, in combination with the ESI or APCI flange, forms the atmospheric pressure region of the API source.

See also atmospheric pressure ionization (API).

API stack Consists of the components of the API source that are held under vacuum and includes the API spray shield, API ion transfer capillary, API tube lens, skimmer, the ion transfer capillary mount, and the tube lens and skimmer mount.

See also atmospheric pressure ionization (API) and API source.

API tube lens A lens in the API source that separates ions from neutral particles as they leave the ion transfer capillary. A potential applied to the tube lens focuses the ions toward the opening of the skimmer and helps to dissociate adduct ions.

See also API tube lens offset voltage, API source, API ion transfer capillary, and adduct ion.

API tube lens and skimmer mount A mount that attaches to the heated capillary mount. The tube lens and skimmer attach to the tube lens and skimmer mount.

API tube lens offset voltage A DC voltage applied to the tube lens. The value is normally tuned for a specific compound.

See also API tube lens, adduct ion, and source CID.

AP-MALDI See atmospheric pressure matrix-assisted laser desorption/ionization (AP-MALDI).

APPI See Atmospheric Pressure Photoionization (APPI).

ASCII American Standard Code for Information Interchange

atmospheric pressure chemical ionization (APCI) A soft ionization technique done in an ion source operating at atmospheric pressure. Electrons from a corona discharge initiate the process by ionizing the mobile phase vapor molecules. A reagent gas forms, which efficiently produces positive and negative ions of the analyte through a complex series of chemical reactions.

See also electrospray ionization (ESI).

atmospheric pressure ionization (API) Ionization performed at atmospheric pressure by using atmospheric pressure chemical ionization (APCI), electrospray ionization (ESI), or nanospray ionization (NSI).

atmospheric pressure matrix-assisted laser desorption/ionization (AP-MALDI) Matrix-assisted laser desorption/ionization in which the sample target is at atmospheric pressure.

See also matrix-assisted laser desorption/ionization (MALDI).

Atmospheric Pressure Photoionization (APPI) A soft ionization technique in which an ion is generated from a molecule when it interacts with a photon from a light source.

atomic mass unit Atomic Mass Unit (u) defined by taking the mass of one atom of carbon12 as being 12u; unit of mass for expressing masses of atoms or molecules.

Automatic Gain Control™ (AGC) Sets the ion injection time to maintain the optimum quantity of ions for each scan. With AGC on, the scan function consists of a prescan and an analytical scan.

See also ion injection time.

auxiliary gas The outer-coaxial gas (nitrogen) that assists the sheath (inner-coaxial) gas in dispersing and/or evaporating sample solution as the sample solution exits the APCI, ESI, or H-ESI nozzle.

auxiliary gas flow rate The relative rate of flow of auxiliary gas (nitrogen) into the API source reported in arbitrary units.

auxiliary gas inlet An inlet in the API probe where auxiliary gas is introduced into the probe.

See also auxiliary gas and atmospheric pressure ionization (API).

auxiliary gas plumbing The gas plumbing that delivers outer coaxial nitrogen gas to the ESI or APCI nozzle.

auxiliary gas valve A valve that controls the flow of auxiliary gas into the API source.

B

b bit

B byte (8 b)

baud rate data transmission speed in events per second

BTU British thermal unit, a unit of energy

C

°C degrees Celsius

CE central electrode (of the Orbitrap analyzer);

European conformity. Mandatory European marking for certain product groups to indicate conformity with essential health and safety requirements set out in European Directives.

cfm cubic feet per minute

chemical ionization (CI) The formation of new ionized species when gaseous molecules interact with ions. The process can involve transfer of an electron, proton, or other charged species between the reactants.

chemical ionization (CI) plasma The collection of ions, electrons, and neutral species formed in the ion source during chemical ionization.

See also chemical ionization (CI).

CI See chemical ionization (CI).

CID See collision-induced dissociation (CID).

cm centimeter

cm^3 cubic centimeter

collision gas A neutral gas used to undergo collisions with ions.

collision-induced dissociation (CID) An ion/neutral process in which an ion is dissociated as a result of interaction with a neutral target species.

consecutive reaction monitoring (CRM) scan type A scan type with three or more stages of mass analysis and in which a particular multi-step reaction path is monitored.

Convectron™ gauge A thermocouple bridge gauge that is sensitive to the pressure as well as the thermal conductivity of the gas used to measure pressures between X and Y.

corona discharge In the APCI source, an electrical discharge in the region around the corona discharge needle that ionizes gas molecules to form a chemical ionization (CI) plasma, which contains CI reagent ions.

See also chemical ionization (CI) plasma and atmospheric pressure chemical ionization (APCI).

CPU central processing unit (of a computer)

CRM See consecutive reaction monitoring (CRM) scan type.

C-Trap curved linear trap

<Ctrl> control key on the terminal keyboard

D

d depth

Da dalton

DAC digital-to-analog converter

damping gas Helium gas introduced into the ion trap mass analyzer that slows the motion of ions entering the mass analyzer so that the ions can be trapped by the RF voltage fields in the mass analyzer.

DART Direct Analysis in Real Time

data-dependent scan A scan mode that uses specified criteria to select one or more ions of interest on which to perform subsequent scans, such as MS/MS or ZoomScan.

DC direct current

divert/inject valve A valve on the mass spectrometer that can be plumbed as a divert valve or as a loop injector.

DS data system

DSP digital signal processor

E

ECD See electron capture dissociation (ECD).

EI electron ionization

electron capture dissociation (ECD) A method of fragmenting gas phase ions for tandem mass spectrometric analysis. ECD involves the direct introduction of low energy electrons to trapped gas phase ions.

See also electron transfer dissociation (ETD) and infrared multiphoton dissociation (IRMPD).

electron multiplier A device used for current amplification through the secondary emission of electrons. Electron multipliers can have a discrete dynode or a continuous dynode.

electron transfer dissociation (ETD) A method of fragmenting peptides and proteins. In electron transfer dissociation (ETD), singly charged reagent anions transfer an electron to multiply protonated peptides within the ion trap mass analyzer. This leads to a rich ladder of sequence ions derived from cleavage at the amide groups along the peptide backbone. Amino acid side chains and important modifications such as phosphorylation are left intact.

See also fluoranthene.

electrospray ionization (ESI) A type of atmospheric pressure ionization that is currently the softest ionization technique available to transform ions in solution into ions in the gas phase.

EMBL European Molecular Biology Laboratory

<Enter> Enter key on the terminal keyboard

ESD ElectroStatic Discharge. Discharge of stored static electricity that can damage electronic equipment and impair electrical circuitry, resulting in complete or intermittent failures.

ESI See electrospray ionization (ESI).

ESI flange A flange that holds the ESI probe in position next to the entrance of the heated capillary, which is part of the API stack. The ESI flange also seals the atmospheric pressure region of the API source and, when it is in the engaged position against the spray shield, compresses the high-voltage safety-interlock switch.

ESI probe A probe that produces charged aerosol droplets that contain sample ions. The ESI probe is typically operated at liquid flows of 1 µL/min to 1 mL/min without splitting. The ESI probe includes the ESI manifold, sample tube, nozzle, and needle.

ESI source Contains the ESI probe and the API stack.

See also electrospray ionization (ESI), ESI probe, and API stack.

ESI spray current The flow of charged particles in the ESI source. The voltage on the ESI spray needle supplies the potential required to ionize the particles.

ESI spray voltage The high voltage that is applied to the spray needle in the ESI source to produce the ESI spray current. In ESI, the voltage is applied to the spray liquid as it emerges from the nozzle.

See also ESI spray current.

ETD See electron transfer dissociation (ETD).

eV Electron Volt. The energy gained by an electron that accelerates through a potential difference of one volt.

Extensible Markup Language See XML (Extensible Markup Language).

external lock mass A lock that is analyzed in a separate MS experiment from your sample. If you need to run a large number of samples, or if accurate mass samples will be intermingled with standard samples, you might want to use external lock masses. These allow more rapid data acquisition by eliminating the need to scan lock masses during each scan.

See also internal lock mass.

F

f femto (10^{-15})

°F degrees Fahrenheit

***.fasta* file** extension of a SEQUEST™ search database file

ft foot

Fast Fourier Transform (FFT) An algorithm that performs a Fourier transformation on data. A Fourier transform is the set of mathematical formulae by which a time function is converted into a frequency-domain function and the converse.

FFT See Fast Fourier Transform (FFT).

fluoranthene A reagent anion that is used in an electron transfer dissociation (ETD) experiment.

firmware Software routines stored in read-only memory. Startup routines and low-level input/output instructions are stored in firmware.

forepump The pump that evacuates the foreline. A rotary-vane pump is a type of forepump.

Fourier Transform - Ion Cyclotron Resonance Mass Spectrometry (FT-ICR MS) A technique that determines the mass-to-charge ratio of an ion by measuring its cyclotron frequency in a strong magnetic field.

fragment ion A charged dissociation product of an ionic fragmentation. Such an ion can dissociate further to form other charged molecular or atomic species of successively lower formula weights.

fragmentation The dissociation of a molecule or ion to form fragments, either ionic or neutral. When a molecule or ion interacts with a particle (electron, ion, or neutral species) the molecule or ion absorbs energy and can subsequently fall apart into a series of charged or neutral fragments. The mass spectrum of the fragment ions is unique for the molecule or ion.

FT Fourier Transformation

FT-ICR MS See Fourier Transform - Ion Cyclotron Resonance Mass Spectrometry (FT-ICR MS).

FTMS Fourier Transformation Mass Spectroscopy

full-scan type Provides a full mass spectrum of each analyte or parent ion. With the full-scan type, the mass analyzer is scanned from the first mass to the last mass without interruption. Also known as single-stage full-scan type.

FWHM Full Width at Half Maximum

G

g gram

G Gauss; giga (10^9)

GC gas chromatograph; gas chromatography

GC/MS gas chromatography / mass spectrometer

GUI graphical user interface

H

h hour

h height

handshake A signal that acknowledges that communication can take place.

HCD See higher energy collision-induced dissociation (HCD).

header information Data stored in each data file that summarizes the information contained in the file.

H-ESI probe Heated-electrospray ionization (H-ESI) converts ions in solution into ions in the gas phase by using electrospray ionization (ESI) in combination with heated auxiliary gas.

higher energy collision-induced dissociation (HCD)

Collision-induced dissociation that occurs in the HCD cell of the Orbitrap mass analyzer. The HCD cell consists of a straight multipole mounted inside a collision gas-filled tube. A voltage offset between C-Trap and HCD cell accelerates parent ions into the collision gas inside the HCD cell, which causes the ions to fragment into product ions. The product ions are then returned to the Orbitrap analyzer for mass analysis. HCD produces triple quadrupole-like product ion mass spectra.

high performance liquid chromatography (HPLC)

Liquid chromatography in which the liquid is driven through the column at high pressure. Also known as high pressure liquid chromatography.

HPLC See high performance liquid chromatography (HPLC).

HV high voltage

Hz hertz (cycles per second)

I

ICR ion cyclotron resonance

ID inside diameter

IEC International Electrotechnical Commission

IEEE Institute of Electrical and Electronics Engineers

in. inch

infrared multiphoton dissociation (IRMPD) In infrared multiphoton dissociation (IRMPD), multiply charged ions consecutively absorb photons emitted by a infrared laser until the vibrational excitation is sufficient for their fragmentation. The fragments continue to pick up energy from the laser pulse and fall apart further to ions of lower mass.

See also electron capture dissociation (ECD).

instrument method A set of experiment parameters that define Xcalibur operating settings for the autosampler, liquid chromatograph (LC), mass spectrometer, divert valve, syringe pump, and so on. Instrument methods are saved as file type .meth.

internal lock mass A lock that is analyzed during the same MS experiment as your sample and is contained within the sample solution or infused into the LC flow during the experiment. Internal lock masses provide the most accurate corrections to the data.

See also external lock mass.

I/O input/output

ion gauge Measures the pressure in the mass analyzer region (high vacuum region) of the vacuum manifold.

ion injection time The amount of time that ions are allowed to accumulate in the ion trap mass analyzer when AGC is off. With AGC on, the ion injection time is set automatically (up to the set maximum ion injection time) based on the AGC target value.

See also: Automatic Gain Control™ (AGC).

ion optics Focuses and transmits ions from the API source to the mass analyzer.

ion source A device that converts samples to gas-phase ions.

ion sweep cone A removable cone-shaped metal cover that fits on top of the API ion transfer capillary and acts as a physical barrier to protect the entrance of the capillary.

ion sweep gas Extra nitrogen gas that flows along the axis of the API ion transfer capillary (between the ion sweep cone and the capillary block) towards the API spray. The sweep gas flow is thus countercurrent to the flow of the ions.

See also ion sweep gas pressure.

ion sweep gas pressure The rate of flow of the sweep gas (nitrogen) into the API source. A measurement of the relative flow rate (in arbitrary units) to provide the required flow of nitrogen gas out from the Ion Sweep cone towards the API spray.

See also ion sweep gas.

IRMPD See infrared multiphoton dissociation (IRMPD).

K

k kilo (10^3, 1000)

K kilo (2^{10}, 1024)

KEGG Kyoto Encyclopedia of Genes and Genomes

kg kilogram

L

l length

L liter

LAN local area network

lb pound

LC See liquid chromatography (LC).

LC/MS See liquid chromatography / mass spectrometry (LC/MS).

LED light-emitting diode

LHe liquid helium

liquid chromatography (LC) A form of elution chromatography in which a sample partitions between a stationary phase of large surface area and a liquid mobile phase that percolates over the stationary phase.

liquid chromatography / mass spectrometry (LC/MS) An analytical technique in which a high-performance liquid chromatograph (LC) and a mass spectrometer (MS) are combined.

LN2 liquid nitrogen

lock mass A known reference mass in the sample that is used to correct the mass spectral data in an accurate mass experiment and used to perform a real-time secondary mass calibration that corrects the masses of other peaks in a scan. Lock masses with well-defined, symmetrical peaks work best. You can choose to use internal lock mass or external lock mass.

log file A text file, with a .log file extension, that is used to store lists of information.

M

μ micro (10^{-6})

m meter; milli (10^{-3})

M mega (10^6)

M^+ molecular ion

MALDI See matrix-assisted laser desorption/ionization (MALDI).

matrix-assisted laser desorption/ionization (MALDI) A method of ionizing proteins where a direct laser beam is used to facilitate vaporization and ionization while a matrix protects the biomolecule from being destroyed by the laser.

MB Megabyte (1 048 576 bytes)

MH^+ protonated molecular ion

microscan One mass analysis (ion injection and storage or scan-out of ions) followed by ion detection. Microscans are summed, to produce one scan, to improve the signal-to-noise ratio of the mass spectral data. The number of microscans per scan is an important factor in determining the overall scan time.

min minute

mL milliliter

mm millimeter

MRFA A peptide with the amino acid sequence methionine–arginine–phenylalanine–alanine.

MS mass spectrometer; mass spectrometry

MS MS^n power: where n = 1

MS scan modes Scan modes in which only one stage of mass analysis is performed. The scan types used with the MS scan modes are full-scan type and selected ion monitoring (SIM) scan type.

MSDS Material Safety Data Sheet

MS/MS Mass spectrometry/mass spectrometry, or tandem mass spectrometry is an analytical technique that involves two stages of mass analysis. In the first stage, ions formed in the ion source are analyzed by an initial analyzer. In the second stage, the mass-selected ions are fragmented and the resultant ionic fragments are mass analyzed.

MS^n scan mode The scan power equal to 1 to 10, where the scan power is the power *n* in the expression MS^n. MS^n is the most general expression for the scan mode, which can include the following:

- The scan mode corresponding to the one stage of mass analysis in a single-stage full-scan experiment or a selected ion monitoring (SIM) experiment
- The scan mode corresponding to the two stages of mass analysis in a two-stage full-scan experiment or a selected reaction monitoring (SRM) experiment
- The scan mode corresponding to the three to ten stages of mass analysis (n = 3 to n = 10) in a multi-stage full-scan experiment or a consecutive reaction monitoring (CRM) experiment

See also MS scan modes and MS/MS.

multipole A symmetrical, parallel array of (usually) four, six, or eight cylindrical rods that acts as an ion transmission device. An RF voltage and DC offset voltage are applied to the rods to create an electrostatic field that efficiently transmits ions along the axis of the multipole rods.

m/z Mass-to-charge ratio. An abbreviation used to denote the quantity formed by dividing the mass of an ion (in u) by the number of charges carried by the ion. For example, for the ion $C_7H_7^{2+}$, m/z=45.5.

N

n nano (10^{-9})

nanospray ionization (NSI) A type of electrospray ionization (ESI) that accommodates very low flow rates of sample and solvent on the order of 1 to 20 nL/min (for static nanospray) or 100 to 1000 nL/min (for dynamic nanospray).

NCBI National Center for Biotechnology Information (USA)

NIST National Institute of Standards and Technology (USA)

NMR Normal Mass Range

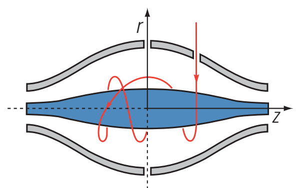
NSI See nanospray ionization (NSI).

O

octapole An octagonal array of cylindrical rods that acts as an ion transmission device. An RF voltage and DC offset voltage applied to the rods create an electrostatic field that transmits the ions along the axis of the octapole rods.

OD outside diameter

Orbitrap mass analyzer The Orbitrap™ mass analyzer consists of a spindle-shape central electrode surrounded by a pair of bell-shaped outer electrodes. Ions inside the mass analyzer orbit in stable trajectories around the central electrode with harmonic oscillations along it.



Two detection electrodes record an image current of the ions as they undergo harmonic oscillations. A Fourier transformation extracts different harmonic frequencies from the image current. An ion's mass-to-charge ratio *m/z* is related to the frequency *f* of its harmonic oscillations and to the instrumental constant *k* by:

$m/z = k/f^2$

OT Orbitrap

See Orbitrap mass analyzer.

OVC outer vacuum case

Ω ohm

P

p pico (10^{-12})

Pa pascal

parent ion An electrically charged molecular species that can dissociate to form fragments. The fragments can be electrically charged or neutral species. A parent ion can be a molecular ion or an electrically charged fragment of a molecular ion. Also called a precursor ion.

parent mass The mass-to-charge ratio of a parent ion. The location of the center of a target parent-ion peak in mass-to-charge ratio (m/z) units. Also known as precursor mass.

See also: parent ion.

PCB printed circuit board

PDA detector Photodiode Array detector is a linear array of discrete photodiodes on an integrated circuit chip. It is placed at the image plane of a spectrometer to allow a range of wavelengths to be detected simultaneously.

PE protective earth

PID proportional / integral / differential

P/N part number

p-p peak-to-peak voltage

ppm parts per million

PQD pulsed-Q dissociation

precursor ion An electrically charged molecular species that can dissociate to form fragments. The fragments can be electrically charged or neutral species. A precursor ion (PR) can be a molecular ion or an electrically charged fragment of a molecular ion. Also known as parent ion.

precursor mass Mass of the corresponding precursor (or parent) ion or molecule.

psig pounds per square inch, gauge

PTM posttranslational modification

pulsed Q dissociation (PQD) Collision-induced dissociation that involves precursor ion activation at high Q, a time delay to allow the precursor to fragment, and then a rapid pulse to low Q where all fragment ions are trapped. The fragment ions can then be scanned out of the ion trap mass analyzer and detected. PQD eliminates the “1/3 Rule” low mass cut-off for MS/MS data.

Q

quadrupole A symmetrical, parallel array of four hyperbolic rods that acts as a mass analyzer or an ion transmission device. As a mass analyzer, one pair of opposing rods has an oscillating radio frequency (RF) voltage superimposed on a positive direct current (DC) voltage. The other pair has a negative DC voltage and an RF voltage that is 180 degrees out of phase with the first pair of rods. This creates an electrical field (the quadrupole field) that efficiently transmits ions of selected mass-to-charge ratios along the axis of the quadrupole rods.

R

RAM random access memory

raw data Uncorrected liquid chromatograph and mass spectrometer data obtained during an acquisition. Xcalibur and Xcalibur-based software store this data in a file that has a .raw file extension.

resolution The ability to distinguish between two points on the wavelength or mass axis.

retention time (RT) The time after injection at which a compound elutes. The total time that the compound is retained on the chromatograph column.

RF radio frequency

RF lens A multipole rod assembly that is operated with only radio frequency (RF) voltage on the rods. In this type of device, virtually all ions have stable trajectories and pass through the assembly.

RF voltage An AC voltage of constant frequency and variable amplitude that is applied to the ring electrode or endcaps of the mass analyzer or to the rods of a multipole. Because the frequency of this AC voltage is in the radio frequency (RF) range, it is referred to as RF voltage.

RMS root mean square

ROM read-only memory

rotary-vane pump A mechanical vacuum pump that establishes the vacuum necessary for the proper operation of the turbomolecular pump. (Also called a roughing pump or forepump.)

RS-232 An accepted industry standard for serial communication connections. This Recommended Standard (RS) defines the specific lines and signal characteristics used by serial communications controllers to standardize the transmission of serial data between devices.

RT An abbreviated form of the phrase *retention time (RT)*. This shortened form is used to save space when the retention time (in minutes) is displayed in a header, for example, RT: 0.00-3.75.

S

s second

scan mode and scan type combinations A function that coordinates the three processes in the MS detector: ionization, mass analysis, and ion detection. You can combine the various scan modes and scan types to perform a wide variety of experiments.

selected ion monitoring (SIM) scan type A scan type in which the mass spectrometer acquires and records ion current at only one or a few selected mass-to-charge ratio values.

See also selected reaction monitoring (SRM) scan type.

selected reaction monitoring (SRM) scan type A scan type with two stages of mass analysis and in which a particular reaction or set of reactions, such as the fragmentation of an ion or the loss of a neutral moiety, is monitored. In SRM a limited number of product ions is monitored.

SEM secondary electron multiplier

Serial Peripheral Interface (SPI) hardware and firmware communications protocol

serial port An input/output location (channel) for serial data transmission.

sheath gas The inner coaxial gas (nitrogen), which is used in the API source to help nebulize the sample solution into a fine mist as the sample solution exits the ESI or APCI nozzle.

sheath gas flow rate The rate of flow of sheath gas into the API source. A measurement of the relative flow rate (in arbitrary units) that needs to be provided at the sheath gas inlet to provide the required flow of sheath gas to the ESI or APCI nozzle.

sheath gas inlet An inlet in the API probe where sheath gas is introduced into the probe.

sheath gas plumbing The gas plumbing that delivers sheath gas to the ESI or APCI nozzle.

sheath gas pressure The rate of flow of sheath gas (nitrogen) into the API source. A measurement of the relative flow rate (in arbitrary units) that needs to be provided at the sheath gas inlet to provide the required flow of inner coaxial nitrogen gas to the ESI or APCI nozzle. A software-controlled proportional valve regulates the flow rate.

See also sheath gas.

sheath gas valve A valve that controls the flow of sheath gas into the API source. The sheath gas valve is controlled by the data system.

signal-to-noise ratio (S/N) The ratio of the signal height (S) to the noise height (N). The signal height is the baseline corrected peak height. The noise height is the peak-to-peak height of the baseline noise.

SIM See selected ion monitoring (SIM) scan type.

skimmer A vacuum baffle between the higher pressure capillary-skimmer region and the lower pressure region. The aperture of the skimmer is offset with respect to the bore of the ion transfer capillary.

source CID A technique for fragmenting ions in an atmospheric pressure ionization (API) source. Collisions occur between the ion and the background gas, which increase the internal energy of the ion and stimulate its dissociation.

SPI See Serial Peripheral Interface (SPI).

SRM See selected reaction monitoring (SRM) scan type.

sweep gas Nitrogen gas that flows out from behind the sweep cone in the API source. Sweep gas aids in solvent declustering and adduct reduction.

See also sweep gas flow rate.

sweep gas flow rate The rate of flow of sweep gas into the API source. A measurement of the relative flow rate (in arbitrary units) to provide the required flow of nitrogen gas to the sweep cone of the API source.

See also sweep gas.

syringe pump A device that delivers a solution from a syringe at a specified rate.

T

T Tesla

target compound A compound that you want to identify or quantitate or that a specific protocol (for example, an EPA method) requires that you look for. Target compounds are also called analytes, or target analytes.

TIC See total ion current (TIC).

TMP See turbomolecular pump.

Torr A unit of pressure, equal to 1 mm of mercury and 133.32 Pa.

total ion current (TIC) The sum of the ion current intensities across the scan range in a mass spectrum.

tube lens offset The voltage offset from ground that is applied to the tube lens to focus ions toward the opening of the skimmer.

See also source CID.

Tune Method A defined set of mass spectrometer tune parameters for the ion source and mass analyzer. Tune methods are defined by using the instrument software's tune window and saved as tune file.

A tune method stores tune parameters only. (Calibration parameters are stored separately, not with the tune method.)

tune parameters Instrument parameters whose values vary with the type of experiment.

turbomolecular pump A vacuum pump that provides a high vacuum for the mass spectrometer and detector system.

TWA time weighted average

U

u atomic mass unit

UHV ultra high vacuum

ultra-high performance liquid chromatography (U-HPLC) See high performance liquid chromatography (HPLC).

Ultramark 1621 A mixture of perfluoroalkoxycyclotriphosphazenes used for ion trap calibration and tuning. It provides ESI singly charged peaks at *m/z* 1022.0, 1122.0, 1222.0, 1322.0, 1422.0, 1522.0, 1622.0, 1722.0, 1822.0, and 1921.9.

UMR Universal Mass Range

V

V volt

V AC volts alternating current

V DC volts direct current

vacuum manifold A thick-walled, aluminum chamber with machined flanges on the front and sides and various electrical feedthroughs and gas inlets that encloses the API stack, ion optics, mass analyzer, and ion detection system.

vacuum system Components associated with lowering the pressure within the mass spectrometer. A vacuum system includes the vacuum manifold, pumps, pressure gauges, and associated electronics.

vent valve A valve that allows the vacuum manifold to be vented to air or other gases. A solenoid-operated valve.

W

w width

W watt

WEEE European Union Waste Electrical and Electronic Equipment Directive. Provides guidelines for disposal of electronic waste.

X

XML (Extensible Markup Language) A general-purpose markup language that is used to facilitate the sharing of data across different information systems, particularly via the Internet.

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