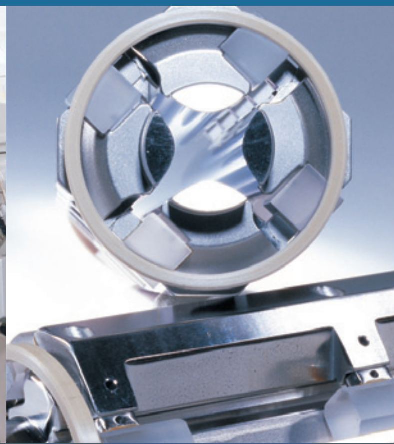
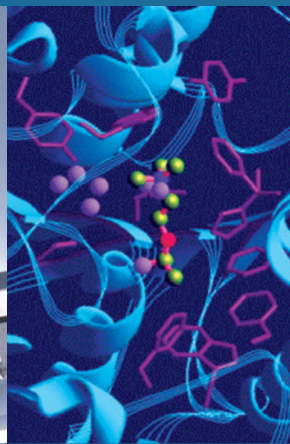
Thermo Fisher Scientific

LTQ Orbitrap XL ETD™

Hardware Manual

Revision A - 1245510





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EG-Konformitätserklärung gemäß ISO/IEC 17050-1:2004
EC Declaration of conformity according to ISO/IEC 17050-1:2004

Name des Herstellers: manufacturers name	Thermo Fisher Scientific
Adresse des Herstellers: manufacturers address	Hanna-Kunath-Strasse 11 28199 Bremen Germany

Der Hersteller erklärt, dass das Produkt
The manufacturer declares that the following product

Name des Produkts: product name	Mass Spectrometer
Modell: model number	LTQ ORBITRAP XL
Produktoptionen: product options	inkl. / incl. ETD

mit den folgenden EG Richtlinien und harmonisierten Standards übereinstimmt:
is in conformity with the following EC Directives and harmonized standards

EMV-Richtlinie EMC Directive **2004/108/EG**	EN 55011 (11.2007) EN 61000-3-2 (10.2006) EN 61000-3-3 (06.2006) EN 61000-4-2 (12.2001) EN 61000-4-3 (12.2006) EN 61000-4-4 (05.2005)	EN 61000-4-5 (06.2007) EN 61000-4-6 (04.2008) EN 61000-4-11 (02.2005) EN 61326-1 (10.2006) + Corr. (06.2008)
Niederspannungsrichtlinie Low Voltage Directive **2006/95/EG**	EN 61010-1 (08.2002)	
Ergänzende Informationen: Complementary information	-	

Bremen, Germany, 16. September 2008

Jörg Behrens
Technischer Leiter
Director of operations

Thermo Fisher
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Declaration of conformity according to ISO/IEC 17050-1:2004

Übereinstimmungserklärung gemäß ISO/IEC 17050-1:2004
Dichiarazione di conformità alla ISO/IEC 17050-1:2004

Manufacturers name Name des Herstellers: nome produttore	Thermo Fisher Scientific
Manufacturers address Adresse des Herstellers: indirizzo produttore	355 River Oaks Parkway San Jose, CA 95134 U.S.A.

declares that the following product
erklärt, dass das Produkt
dichiara che il seguente prodotto

LTQ Orbitrap XL

complies with the following product specifications
mit den folgenden Produktspezifikationen übereinstimmt:
rispetta le seguenti specifiche del prodotto

EMC (emissions) EMV (Störemissionen): EMC (emissioni)	EN 61000-6-3 Störemission (08.02) EN 55022, Kl.B (09.03), EN 61000-3-2 (10.98), EN 61000-3-3 (10.98)
EMC (immunity) EMV (Störfestigkeit): EMC (immunità)	EN 61000-6-2 Störfestigkeit (08.02), EN 61000-4-2 (12.01), -3 (03.03), -4 (07.02), -5 (12.01), -6 (12.01), -11 (12.01), EN 50204 (02.96)
electrical safety Elektrische Sicherheit: sicurezza elettrica	EN 61010-1
complementary information Ergänzende Informationen: informazioni complementari	

This product complies with EMC directive 89/336/EEC and Low Voltage Directive 73/23/EEC.
Dieses Produkt erfüllt die EMV-Richtlinie 89/336/EWG und Niederspannungsrichtlinie 73/23/EWG.
Questo produtto rispetta la direttiva 89/336/EEC e la direttiva 73/23/EEC.

San Jose CA, USA, 8/15/2008

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Regulatory Compliance

Thermo Electron San Jose 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 below.

EMC Directive 89/336/EEC

EMC compliance has been evaluated by TUV Rheinland of North America, Inc..

EN 61000-3-2	1995, A1; 1998, A2; 1998, A14; 2000	EN 61000-4-4 IEC 61000-4-4	1995, A1; 2001, A2; 2001; A2-1995
EN 61000-3-3	1998	EN 61000-4-5	1995, A1; 2001
		IEC 61000-4-5	2005
EN 61326-1	1998, A3	EN 61000-4-6	1996, A1; 2001
		IEC 61000-4-6	2004
EN 61000-4-2	2000	EN 61000-4-11	1994, A1; 2001
IEC 61000-4-2	2001	IEC 61000-4-11	2001-03
FCC Class A, CFR 47 Part 15	2005	CISPR 11	1999, A1; 1999, A2; 2002

Low Voltage Safety Compliance

This device complies with Low Voltage Directive 73/23/EEC and harmonized standard EN 61010-1:2001.

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 Electron. To ensure continued compliance with EMC and safety standards, replacement parts and additional components, options, and peripherals must be ordered from Thermo Electron or one of its authorized representatives.

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Thermo Fisher SCIENTIFIC

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This product is required to comply with the European Union's Waste Electrical & Electronic Equipment (WEEE) Directive 2002/96/EC. It is marked with the following symbol:

Thermo Fisher Scientific has contracted with one or more recycling/disposal companies in each EU Member State, and this product should be disposed of or recycled through them. Further information on Thermo Fisher Scientific's compliance with these Directives, the recyclers in your country, and information on Thermo Fisher Scientific products which may assist the detection of substances subject to the RoHS Directive are available at www.thermo.com/WEEERoHS.

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Read This First

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

About This Guide

This *LTQ Orbitrap XL ETD Hardware Manual* contains a description of the modes of operation and principle hardware components of your LTQ Orbitrap XL ETD instrument. In addition, this manual provides step-by-step instructions for cleaning and maintaining your instrument.

Who Uses This Guide

This *LTQ Orbitrap XL ETD Hardware Manual* is intended for all personnel that need a thorough understanding of the instrument (to perform maintenance or troubleshooting, for example). This manual should be kept near the instrument to be available for quick reference.

Scope of This Guide

This manual includes the following chapters:

- Chapter 1: "Functional Description" describes the principal components of the LTQ Orbitrap XL ETD.
- Chapter 2: "Basic System Operations" provides procedures for shutting down and starting up the LTQ Orbitrap XL ETD.
- Chapter 3: "User Maintenance" outlines the maintenance procedures that you should perform on a regular basis to maintain optimum instrument performance.
- Chapter 4: "Replaceable Parts" lists the replaceable parts for the MS detector and data system.
- Appendix A: "Fluoranthene" describes properties of the reagent that is used in the ETD Module portion of the LTQ Orbitrap XL ETD.

Related Documentation

In addition to this guide, Thermo Fisher Scientific provides the following documents for LTQ Orbitrap XL ETD:

- *LTQ Orbitrap XL / LTQ Orbitrap Discovery Preinstallation Requirements Guide*
- *LTQ Orbitrap XL Getting Started Guide*
- LTQ XL manual set

The software also provides Help.

Contacting Us

There are several ways to contact Thermo Fisher Scientific.

Assistance

For technical support and ordering information, **visit us on the Web**:

www.thermo.com/advancedms

Customer Information Service

cis.thermo-bremen.com is the Customer Information Service site aimed at providing instant access to

- latest software updates
- manuals, application reports, and brochures.

Note Thermo Fisher Scientific recommends that you register with the site as early as possible. ▲

To register, visit register.thermo-bremen.com/form/cis and fill in the registration form. Once your registration has been finalized, you will receive confirmation by e-mail.

Changes to the Manual

To suggest changes to this manual, please send your comments (in German or English) to:

Editors, Technical Documentation
Thermo Fisher Scientific
Hanna-Kunath-Str. 11

28199 Bremen

Germany

`documentation.bremen@thermofisher.com`

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

Typographical Conventions

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

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 on **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

Safety and 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.

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

Notice on Lifting and Handling of Thermo Scientific Instruments

For your safety, and in compliance with international regulations, the physical handling of this Thermo Scientific instrument *requires a team effort* for lifting and/or moving the instrument. This instrument is too heavy and/or bulky for one person alone to handle safely.

Notice on the Proper Use of Thermo Scientific Instruments

In compliance with international regulations: If this instrument is used in a manner not specified by Thermo Fisher Scientific, the protection provided by the instrument could be impaired.

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.

Safety and Special Notices

Note Read and understand the various precautionary notes, signs, and symbols contained inside this manual pertaining to the safe use and operation of this product before using the device. ▲

Make sure you follow the precautionary statements presented in this guide. The safety and other special notices appear different from the main flow of text. Safety and special notices include the following:

Warning Warnings highlight hazards to human beings. Each Warning is accompanied by a Warning symbol. ▲

Caution Cautions highlight information necessary to protect your instrument from damage. ▲

Note Notes highlight information that can affect the quality of your data. In addition, notes often contain information that you might need if you are having trouble. ▲

Identifying Safety Information

The *LTQ Orbitrap XL ETD Hardware Manual* contains precautionary statements that can prevent personal injury, instrument damage, and loss of data if properly followed. Warning symbols alert the user to check for hazardous conditions. These appear throughout the manual, where applicable. The most common warning symbols are:

Warning This general symbol indicates that a hazard is present that could result in injuries if it is not avoided.
The source of danger is described in the accompanying text. ▲

Warning High Voltages capable of causing personal injury are used in the instrument. The instrument must be shut down and disconnected from line power before service is performed. Do not operate the instrument with the top cover off. Do not remove protective covers from PCBs. ▲

Warning Treat heated zones with respect. Parts of the instrument might be very hot and might cause severe burns if touched. Allow hot components to cool before servicing them. ▲

Warning Wear gloves when handling toxic, carcinogenic, mutagenic, or corrosive/irritant chemicals. Use approved containers and procedures for disposal of waste solution. ▲

In addition to the above described, every instrument has specific hazards. So, be sure to read and comply with the precautions described in the subsequent chapters of this guide. They will help ensure the safe, long-term use of your system.

General Safety Precautions

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

- Before plugging in any of the instrument modules or turning on the power, always make sure that the voltage and fuses are set appropriately for your local line voltage.

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

- The supplied power cord must be inserted into a power outlet with a protective earth contact (ground). When using an extension cord, make sure that the cord also has an earth contact.

- Do not change the external or internal grounding connections. Tampering with or disconnecting these connections could endanger you and/or damage the system.

Caution 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. ▲

- Never run the system without the housing on. Permanent damage can occur.

- Do not turn the instrument on if you suspect that it has incurred any kind of electrical damage. Instead, disconnect the power cord and contact a Service Representative for a product evaluation. Do not attempt to use the instrument until it has been evaluated. (Electrical damage may have occurred if the system shows visible signs of damage, or has been transported under severe stress.)

- Damage can also result if the instrument is stored for prolonged periods under unfavorable conditions (e.g., subjected to heat, water, etc.).

- Always disconnect the power cord before attempting any type of maintenance.

- Capacitors inside the instrument may still be charged even if the instrument is turned off.

- Never try to repair or replace any component of the system that is not described in this manual without the assistance of your service representative.

Safety Advice for Possible Contamination

Hazardous Material Might Contaminate Certain Parts of Your System During Analysis.

In order to protect our employees, we ask you to adhere to special precautions when returning parts for exchange or repair.

If hazardous materials have contaminated mass spectrometer parts, Thermo Fisher Scientific can only accept these parts for repair if they have been properly decontaminated. Materials, which due to their structure and the applied concentration might be toxic or which in publications are reported to be toxic, are regarded as hazardous. Materials that will generate synergetic hazardous effects in combination with other present materials are also considered hazardous.

Your signature on the **Repair-Covering letter** confirms that the returned parts have been decontaminated and are free of hazardous materials.

The Repair-Covering letter can be ordered from your service engineer or downloaded from the **Customer Information Service** (**CIS**) site. Please register under http://register.thermo-bremen.com/form/cis.

Parts contaminated by radioisotopes are not subject to return to Thermo Fisher Scientific – either under warranty or the exchange part program. If parts of the system may be possibly contaminated by hazardous material, please make sure the Field engineer is informed before the engineer starts working on the system.

Contents

Figures

Tables

Chapter 1 Functional Description

This chapter provides an overview of the functional elements of the LTQ Orbitrap XL ETD. It contains the following topics:

General Description

LTQ Orbitrap XL ETD is a hybrid mass spectrometer incorporating the LTQ XL™ linear trap, the Orbitrap™ analyzer, and the ETD Module. Figure 1-1 shows a front view of the instrument.

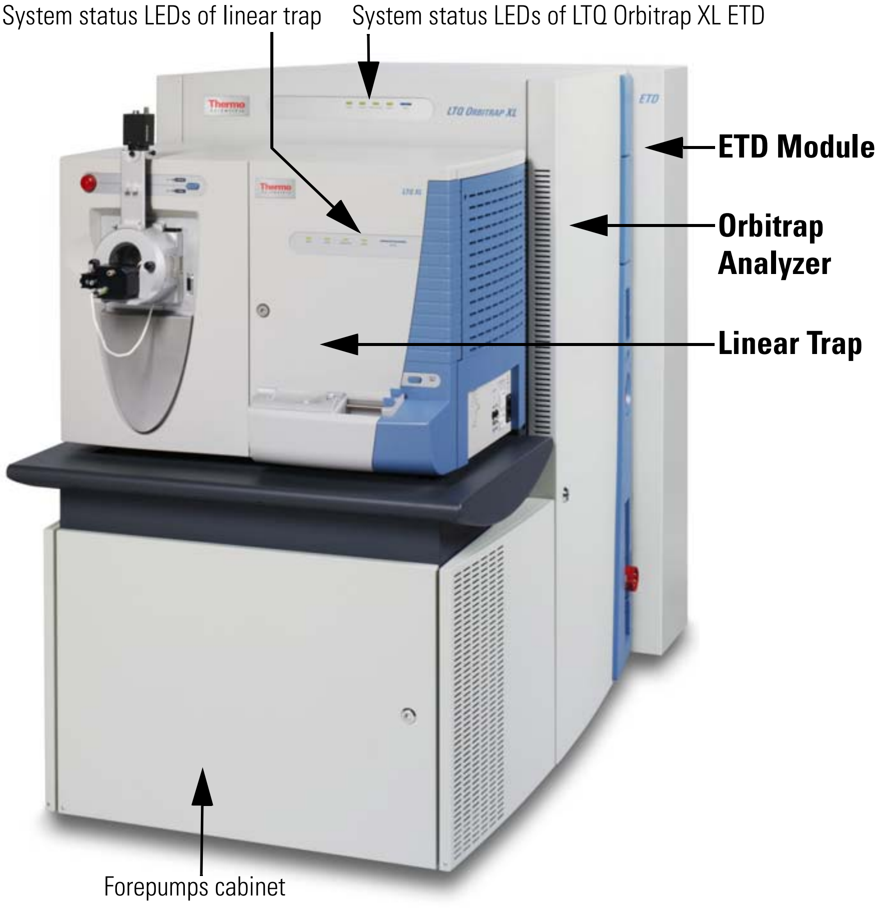


Figure 1-1. LTQ Orbitrap XL ETD front view

The LTQ Orbitrap XL ETD consists of five main components (See Figure 1-2 on page 1-3.), which are described in the following topics:

- A linear ion trap (Thermo Scientific LTQ XL) for sample ionization, selection, fragmentation, and AGC™.
- An intermediate storage device (curved linear trap) that is required for short pulse injection.
- An Orbitrap analyzer for Fourier transformation based analysis.
- A collision cell for performing higher energy CID experiments.
- A reagent ion source for enabling post-translational modification analyses of peptides by Electron Transfer Dissociation.

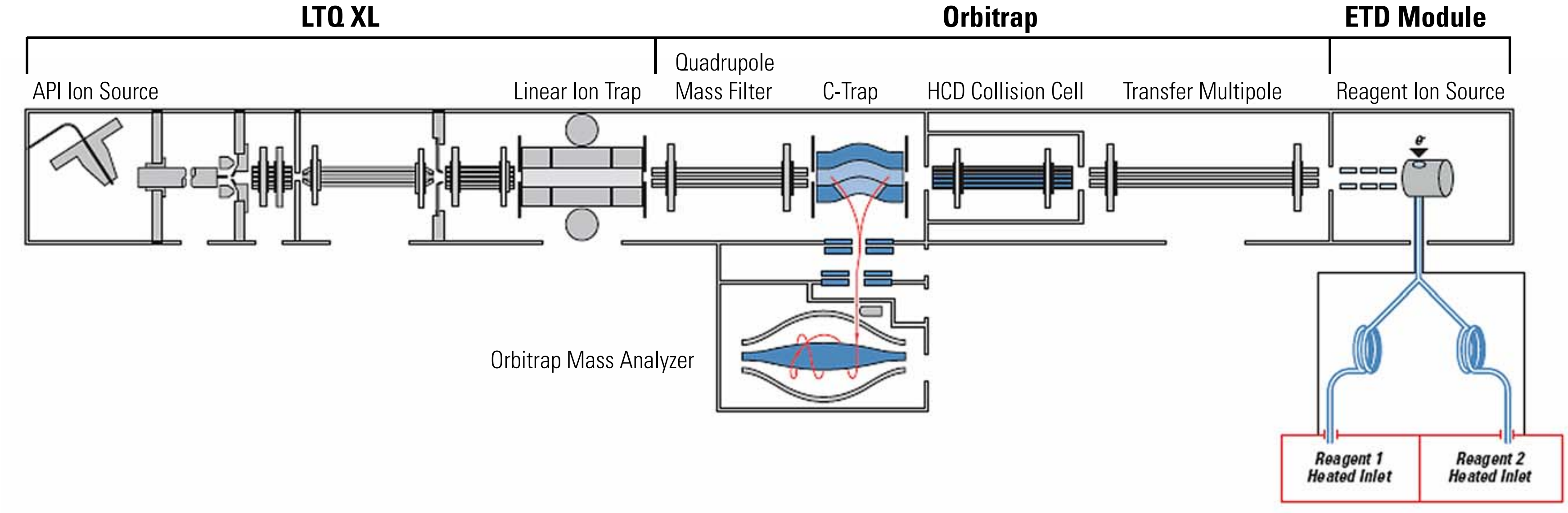


Figure 1-2. Schematical view of the LTQ Orbitrap XL ETD

Note The ETD system is also available as an upgrade on new and existing LTQ Orbitrap (only after upgrade to LTQ Orbitrap XL) and LTQ Orbitrap XL systems. The ETD system is not available for LTQ Orbitrap Discovery systems. ▲

Mechanical Characteristics

Wheels at the bottom side of the instrument facilitate positioning the LTQ Orbitrap XL ETD at the intended place in the laboratory.

The mains inlet as well as a power outlet for peripheral devices are located at the right side of the instrument. The rotary pumps for the vacuum system of the linear trap and the Orbitrap are hidden under the linear trap and accessible from the front. The rotary pump 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 Field Engineers from the top. See Figure 1-3. After removing the cables, the top lid of the ETD Module is also removable to allow accessing its electronic components.

Figure 1-3. Top lid of MS portion opened

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

Specifications

The LTQ Orbitrap XL ETD has the following measuring specifications:

Resolution	60000 (FWHM) @ *m/z* 400 with a scan repetition rate of 1 second Minimum resolution 7500, maximum resolution 100000 @ *m*/z 400
Cycle Time	1 scan at 60000 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, <2 ppm RMS with internal calibration
Dynamic Range	>10000 between mass spectra, >4000 between highest and lowest detectable ion signal in one spectrum
MS/MS	MS/MS and MS^n scan functions

Control Elements

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

System Status LEDs

Figure 1-4 shows the system status LEDs at the front of the instrument. Five LEDs indicate the main functions of the system. (See also Figure 1-5 on page 1-7.) The Power LED is directly controlled by the 3 × 230 V input and all other LEDs are controlled by the power distribution board (Refer to topic "Power Distribution Board" on page 1-52). Table 1-1 explains the function of the various LEDs.

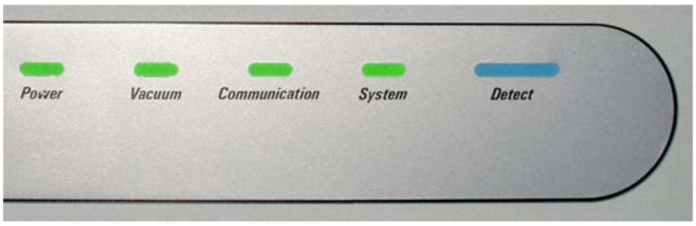


Figure 1-4. System status LEDs

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

Table 1-1. System status LEDs of the LTQ Orbitrap XL ETD

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

*These LEDs are flashing when a system bakeout is performed. See topic "Baking Out the System" on page 3-4.

Control Panels

Figure 1-5 shows the right side of the LTQ Orbitrap XL ETD. Located here are the control panels, switches, and the ports for the external connections (mains supply, gases, Ethernet communication, and cooling water). The ETD Module power panel is also accessible from this side.

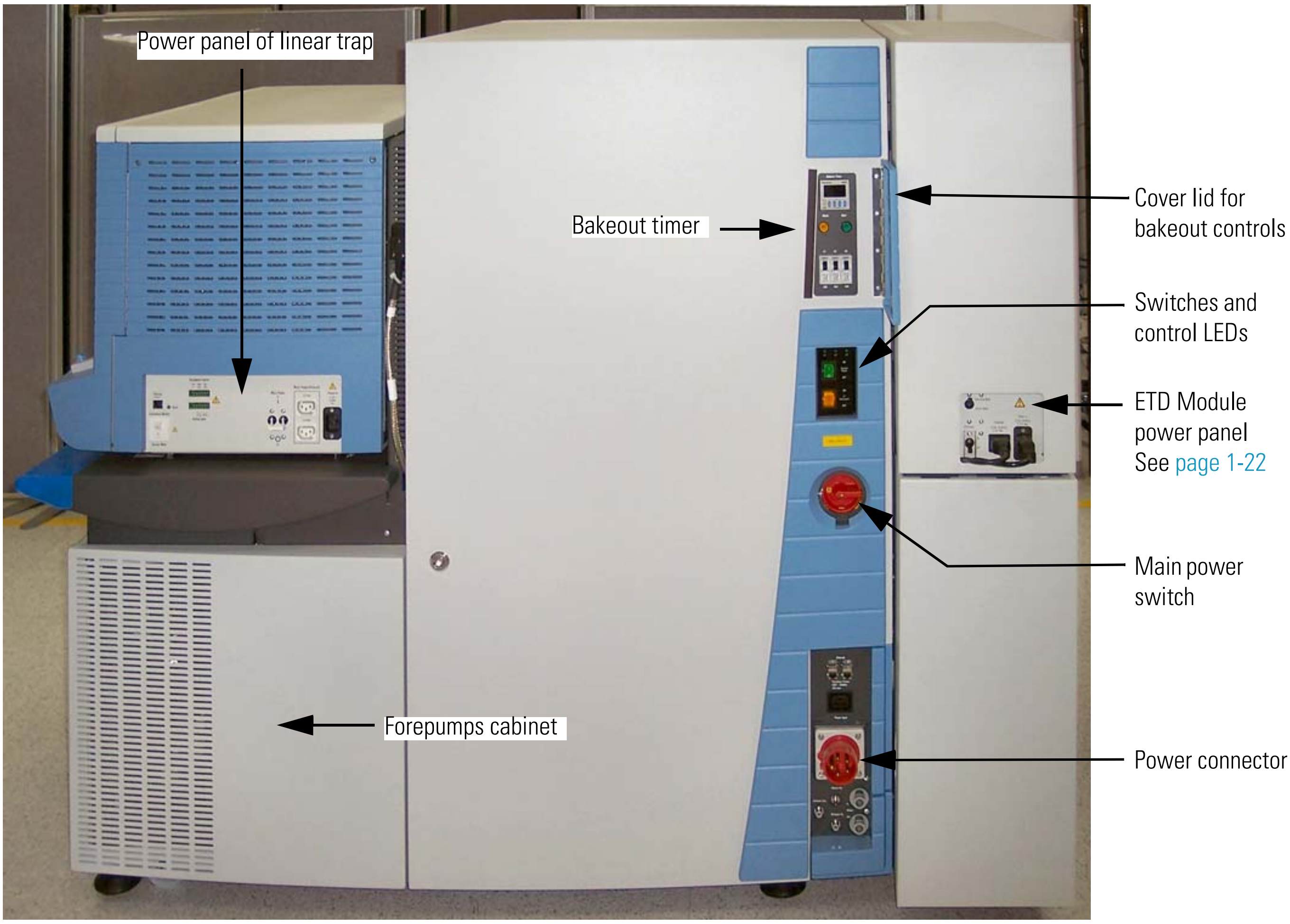


Figure 1-5. Right side of the LTQ Orbitrap XL ETD

For more information about the external connections, refer to topic "External Connections" on page 1-10.

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 1-5 and Figure 1-6 on page 1-8.

The timer allows setting the duration for the bakeout of the system. After the duration is set, the bakeout procedure is started by pressing the green button on the right. A running bakeout procedure can be stopped by pressing the orange button on the left side. For instructions about performing a bakeout, refer to topic "Baking Out the System" on page 3-4.

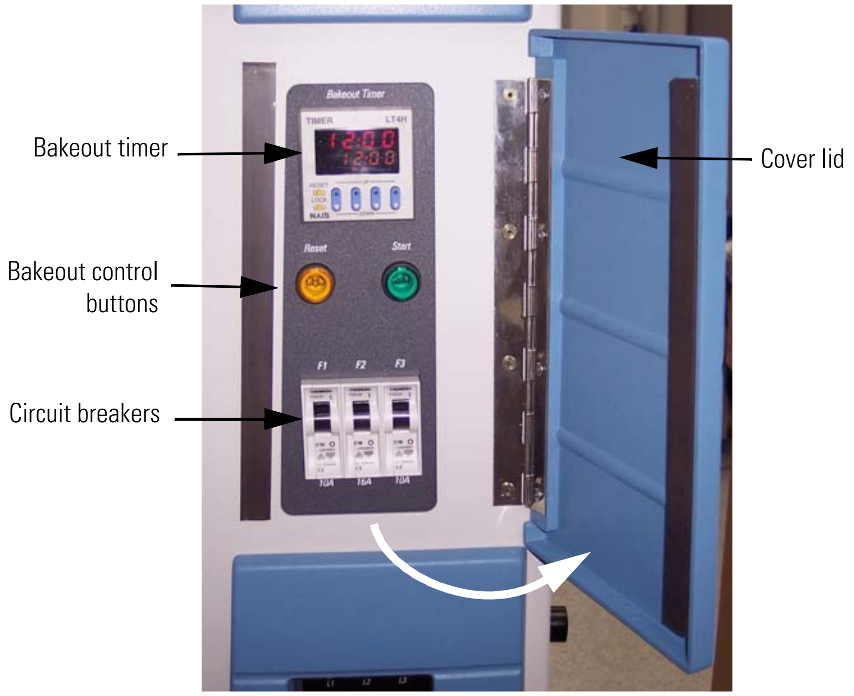


Figure 1-6. Upper control panel

Note The buttons themselves have no indicator function. A running bakeout procedure is indicated by flashing Vacuum and System LEDs at the front side of the instrument. See Figure 1-4 on page 1-6. ▲

Three circuit breakers are located at the bottom of this control panel. Table 1-2 shows the parts of the LTQ Orbitrap XL ETD 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 1-2. Circuit breakers of the LTQ Orbitrap XL ETD

Circuit breaker	Ampere	LED	Instrument parts
F1	10	L1	Power Distribution
F2	16	L2	Linear ion trap
F3	10	L3	Multiple socket outlets (Peripherals, LC, heater, etc.)

Power Control Panel

In addition to the system status LEDs at the front side (see Figure 1-4 on page 1-6), the LTQ Orbitrap XL ETD has three power control LEDs above the Vacuum Pumps switch at the right side. See Figure 1-7. They indicate whether the corresponding circuit breaker is closed and the respective parts of the instrument have power. (See Table 1-2 on page 1-8.)

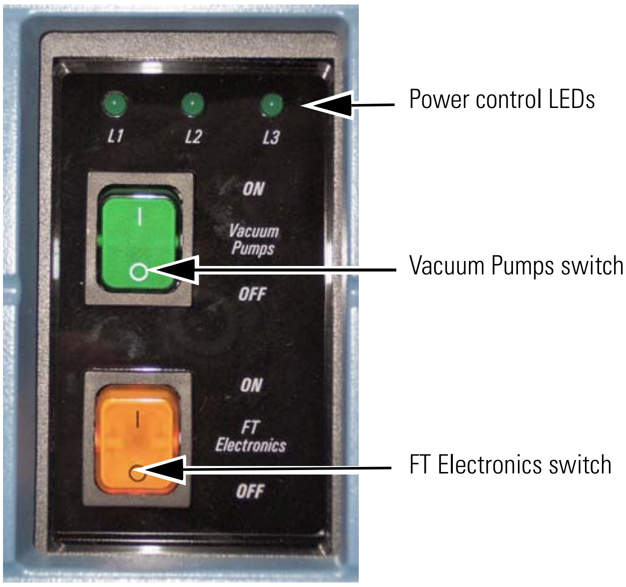


Figure 1-7. Power control panel with power control LEDs and switches

The use of the switches below the power control LEDs changes the working mode of the power distribution. (See topic "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 (Refer to the topic "Power Distribution Board" on page 1-52)
- Pumps (Refer to the topic "Vacuum System" on page 1-28)

- Temperature controller (Refer to the topic "Temperature Controller Board" on page 1-61)

- 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/anti-clockwise to switch on/off the instrument (see Figure 1-8). Placing the main power switch in the Off position turns off all power to the LTQ Orbitrap XL ETD, the linear ion trap, the vacuum pumps, and the ETD Module.

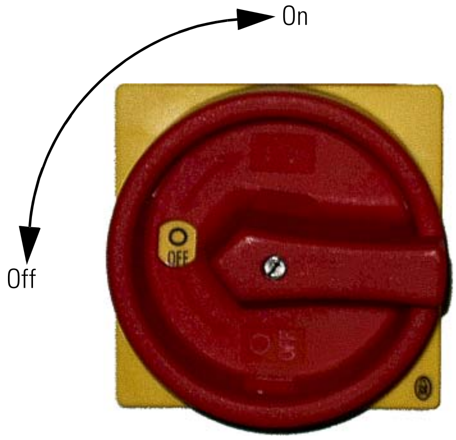


Figure 1-8. Main power switch

Note 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 1-9 on page 1-11 shows the lower right side of the instrument with the external connections for mains supply, gases, cooling water, and Ethernet communication.

The power connector for the mains supply is located on the center. The cooling water ports are located below the power connector. (See also topic "Cooling Water Circuit" on page 1-40.) A Teflon® hose connects the instrument to the nitrogen gas supply. An analogous port is used for the HCD collision gas supply. Metal tubing connects the instrument with the helium gas supply. (See also topic "Gas Supply" on page 1-36.)

Located at the top are two ports for Ethernet cables for connecting the LTQ Orbitrap XL ETD and the linear ion trap via an Ethernet hub with the data system computer.

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

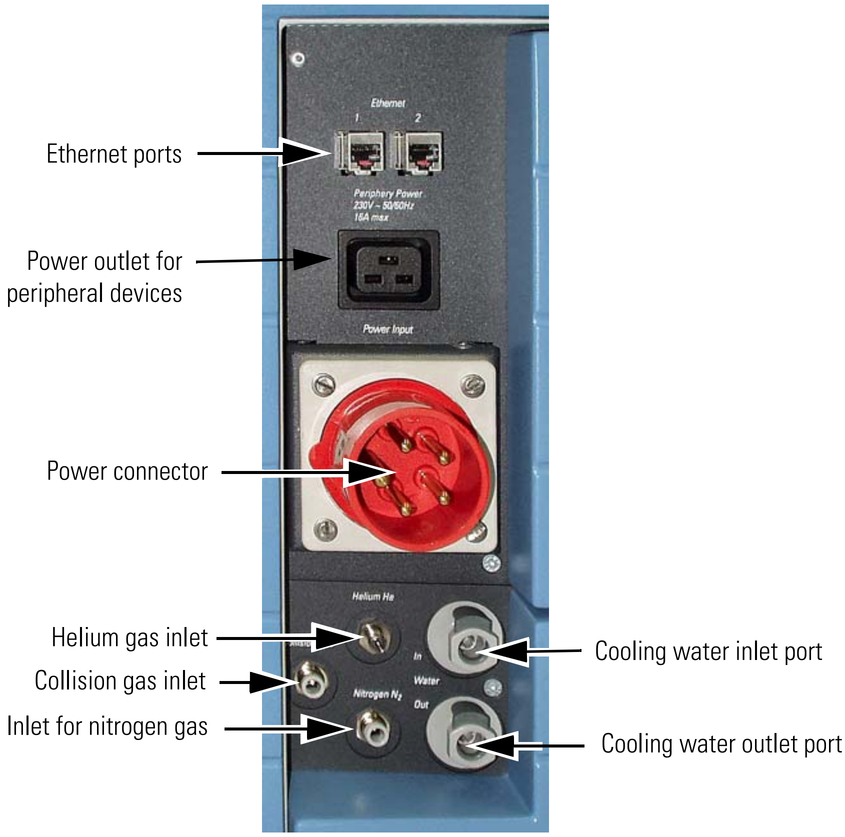


Figure 1-9. External connections to the LTQ Orbitrap XL ETD

The power outlet for peripheral devices is located above the mains supply port. The outlet provides the mains supply for the ETD Module.

Linear Ion Trap

The LTQ Orbitrap XL ETD system can utilize a variety of ionization techniques such as ESI, APCI, or APPI. Maintenance of the 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 1-2 on page 1-3.)

The linear ion trap is an independent MS detector (Thermo Scientific LTQ XL), which can store, isolate, and fragment ions and then send them either to the Orbitrap 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 completely described in the *LTQ XL 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. These features include storage and ejection of all ions, storage of selected masses or mass ranges, as well as ion isolation. Isolated ions can be excited and then fragmented as necessary for MS/MS and MSn 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 1-1 on page 1-2. The table also serves as a housing for the forepumps. See Figure 1-24 on page 1-31. The LTQ Orbitrap XL ETD provides power for the linear ion trap – and for the ETD Module.

The linear ion trap is delivered with power connector, gas lines (He, N_2, and collision gas), and vacuum tube lines extending to the ESI source. On the rear side of the LTQ XL 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 are fixed to the transfer chamber.

Orbitrap Analyzer

This section describes the basic principle of the Orbitrap™ mass analyzer. The heart of the system 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 1-10. The Orbitrap employs electric fields to capture and confine ions.

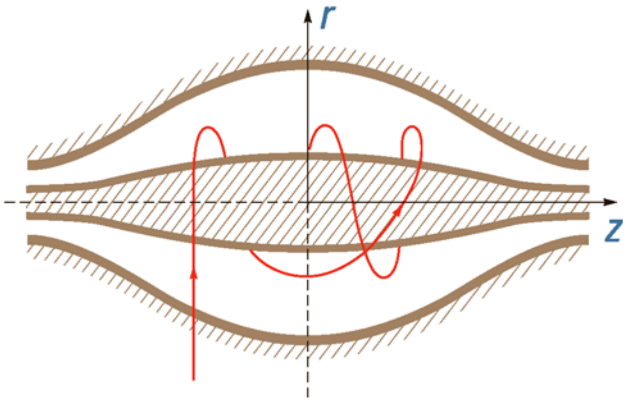


Figure 1-10. Schematical view of the Orbitrap cell and example of a stable ion trajectory

Measuring Principle

In the mass analyzer shown in Figure 1-10, ions rotate on stable trajectories rotate 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/q* and the instrumental constant *k*:

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

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

Curved Linear Trap

On their way from the linear trap to the Orbitrap, ions move through the gas-free RF-only quadrupole into the gas-filled curved linear trap (C-Trap). See Figure 1-11 on page 1-14. Ions in the C-Trap are returned by the trap electrode. Upon their passage, the ions loose enough kinetic energy to prevent them from leaving the C-Trap through the gate. The nitrogen collision gas (bath gas) is used for dissipating the kinetic energy of ions injected from the LTQ XL and for cooling them down to the axis of the curved linear trap.

Voltages on the end apertures of the curved trap (trap and gate apertures) are elevated to provide a potential well along its axis. These voltages may be later ramped up to squeeze ions into a shorter thread along this axis. The RF to the C-Trap ("Main RF") is provided by the CLT RF main board. (See page 1-62.) Trap and gate dc voltages are provided by the ion optic supply board. (See page 1-59.) The RF voltages to the quadrupole mass filter are supplied by the linear trap. High voltages to the lenses are provided by the high voltage power supply board. (See page 1-65.)

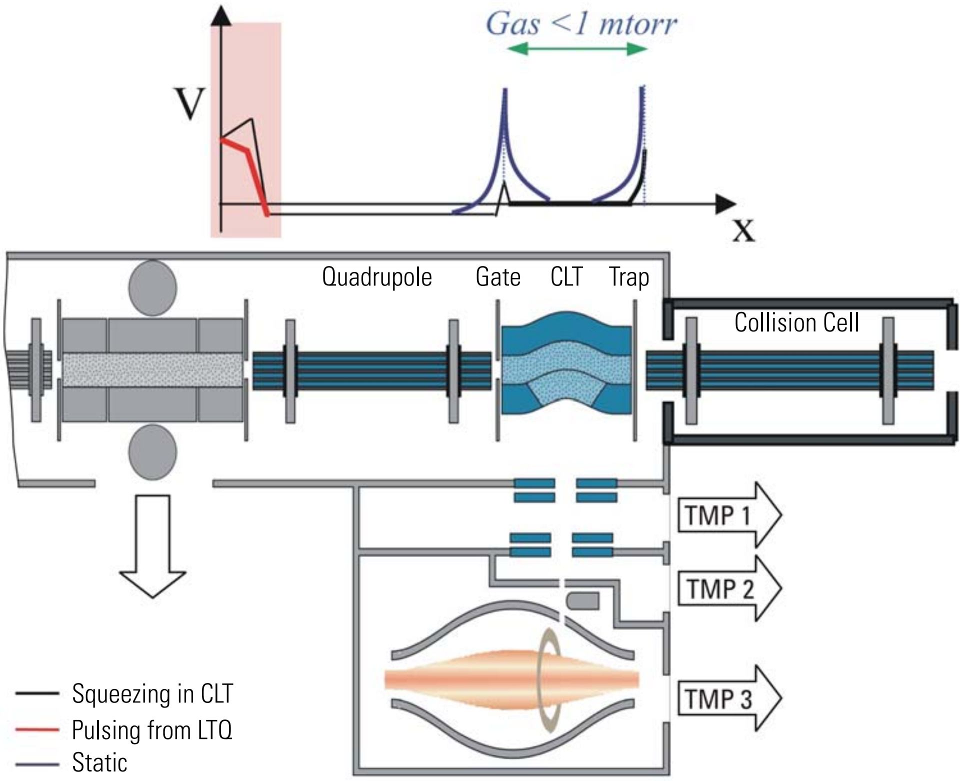


Figure 1-11. Layout of the instrument, also showing the applied voltages

Extraction of Ion Packets

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

Owing to the fast pulsing of ions from the curved trap, ions of each mass-to-charge ratio arrive at the entrance of the Orbitrap 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 at a position offset from its equator (Figure 1-12), these packets start coherent axial oscillations without the need for any additional excitation cycle.

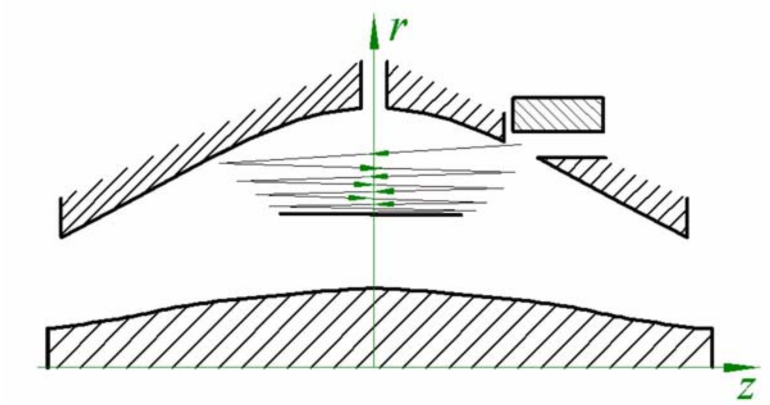


Figure 1-12. Principle of electrodynamic squeezing of ions in the Orbitrap as the field strength is increased

The evolution of an ion packet during the increase of the electric field is shown schematically on Figure 1-12. 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/q) to enter the trap as well. After ions of all m/q have entered the Orbitrap and moved far enough from the outer electrodes, the voltage on the central electrode is kept constant and image current detection takes place.

Ion Detection

During ion detection, both the central electrode and deflector 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 fast Fourier transform algorithm.

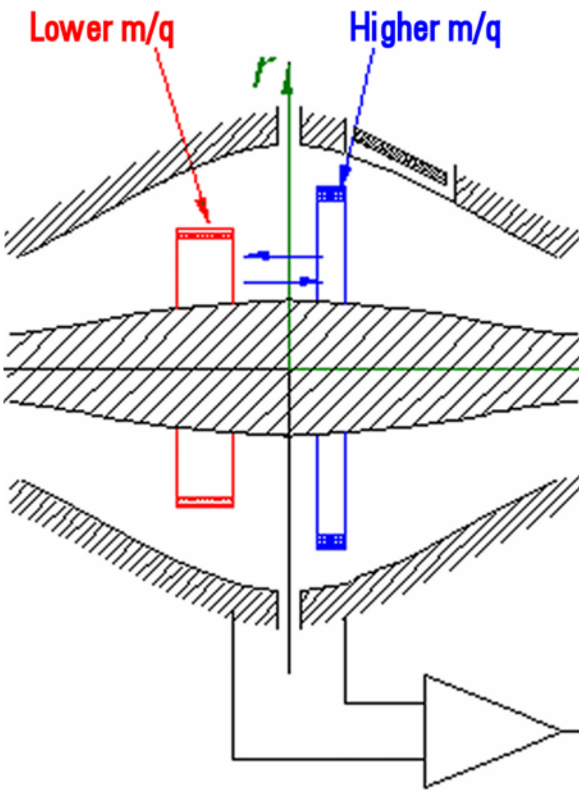


Figure 1-13. Approximate shape of ion packets of different m/q after stabilization of voltages

As mentioned above, stable ion trajectories within the Orbitrap combine axial oscillations along the z-axis with rotation around the central electrode and vibrations in the radial direction. (See Figure 1-10 on page 1-13.) For any given *m/q*, 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/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/q* assumes the shape of a thin ring, with ions uniformly distributed along its circumference. (See Figure 1-13.) 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 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 1-61.

Peltier Cooling

To allow stable operating conditions in the UHV chamber, it can be cooled or heated (outgassing) by means of a Peltier element located on the outside. A second Peltier element is located on the back of the CE power supply board. See Figure 1-41 on page 1-58.

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 LTQ Orbitrap XL ETD. See topic “Cooling Water Circuit” on page 1-40 for further information.

HCD Collision Cell

The collision 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 a collision gas through the open split interface, providing increased gas pressure inside the multipole. The choice of collision gas is independent from the gas in the C-Trap. See topic "Gas Supply" on page 1-36 for details. The front of the tube is equipped with a lens for tuning transmission and ejection to/from the C-Trap. The ion optic supply board provides the voltages for the collision cell. (See page 1-59.)

For HCD (Higher Energy Collisional Dissociation), ions are passed through the C-Trap into the collision cell. The offset between the C-Trap and HCD is used to accelerate the parents into the gas-filled collision cell.

The fragment spectra generated in the collision cell and detected in the Orbitrap show a fragmentation pattern comparable to the pattern of typical collisional quadrupole spectra. See the *LTQ Orbitrap XL Getting Started* manual for more information.

To reduce damping of ions by the collision gas (collisional damping), a potential gradient is applied to the collision cell, such that it transmits ions at a reliable rate. The direction of the gradient (and the voltage offset of the cell) can be switched to allow alternation between positive ion HCD mode, negative ion HCD mode, ETD mode, or auxiliary ion source mode.

Note 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 (i.e. scan to scan) between HCD and ETD fragmentation, thus making comparative measurements possible. When compared with the standard LTQ Orbitrap XL, HCD performance is not in any way compromised by the addition of the ETD Module. ▲

ETD System

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 deliver 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 type 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.

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 collision cell, and the C-Trap. (See Figure 1-2 on page 1-3.)

The reagent ions pass a quadrupole mass filter[1] between C-Trap and linear trap. This ion guide works as a low pass mass filter to remove the adduct of the fluoranthene radical and molecular nitrogen at *m/z* 216. This adduct favors 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 (if mass resolution and accuracy are important).

ETD Module

Figure 1-14 on page 1-20 shows the rear side of the ETD Module. It is mounted to the rear side of the instrument. 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.

[1] The linear trap provides the voltages for the quadrupole mass filter.

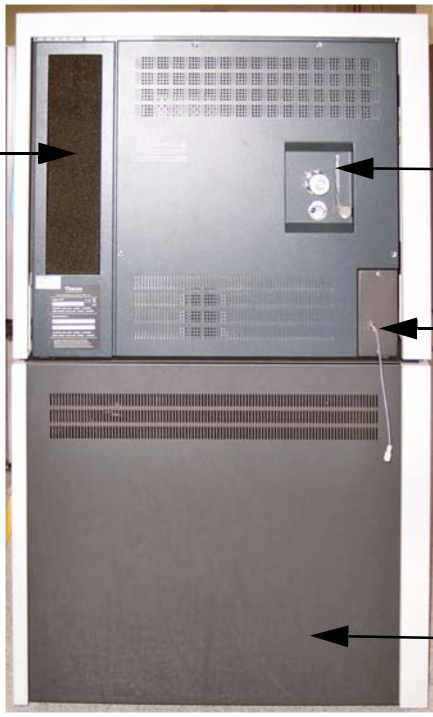
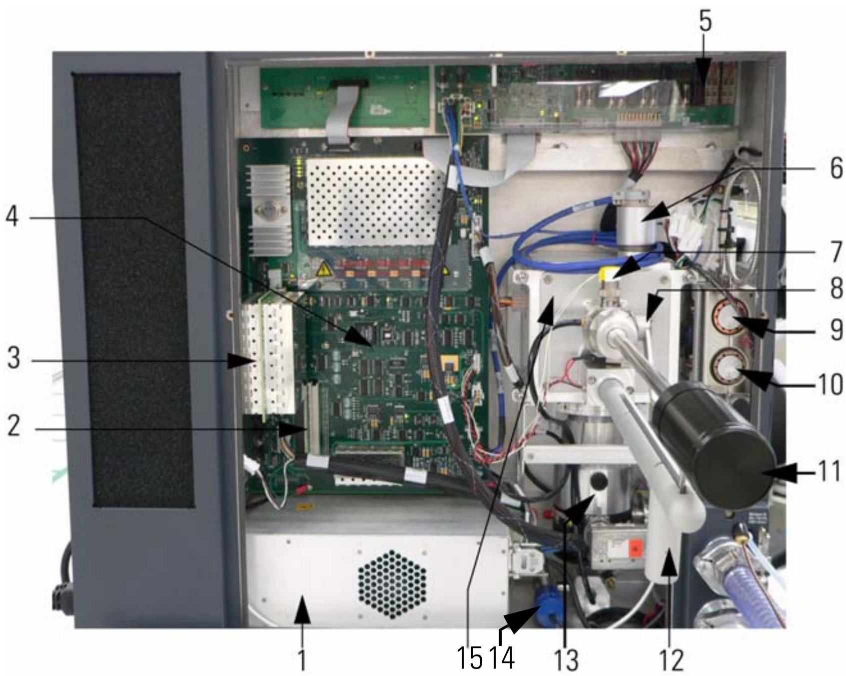


Figure 1-14. LTQ Orbitrap XL ETD, rear side



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=turbopump, 14=Convectron gauge, 15=vacuum manifold (contains ion source and ion volume)

Figure 1-15. Rear view of the ETD Module, with major component locations

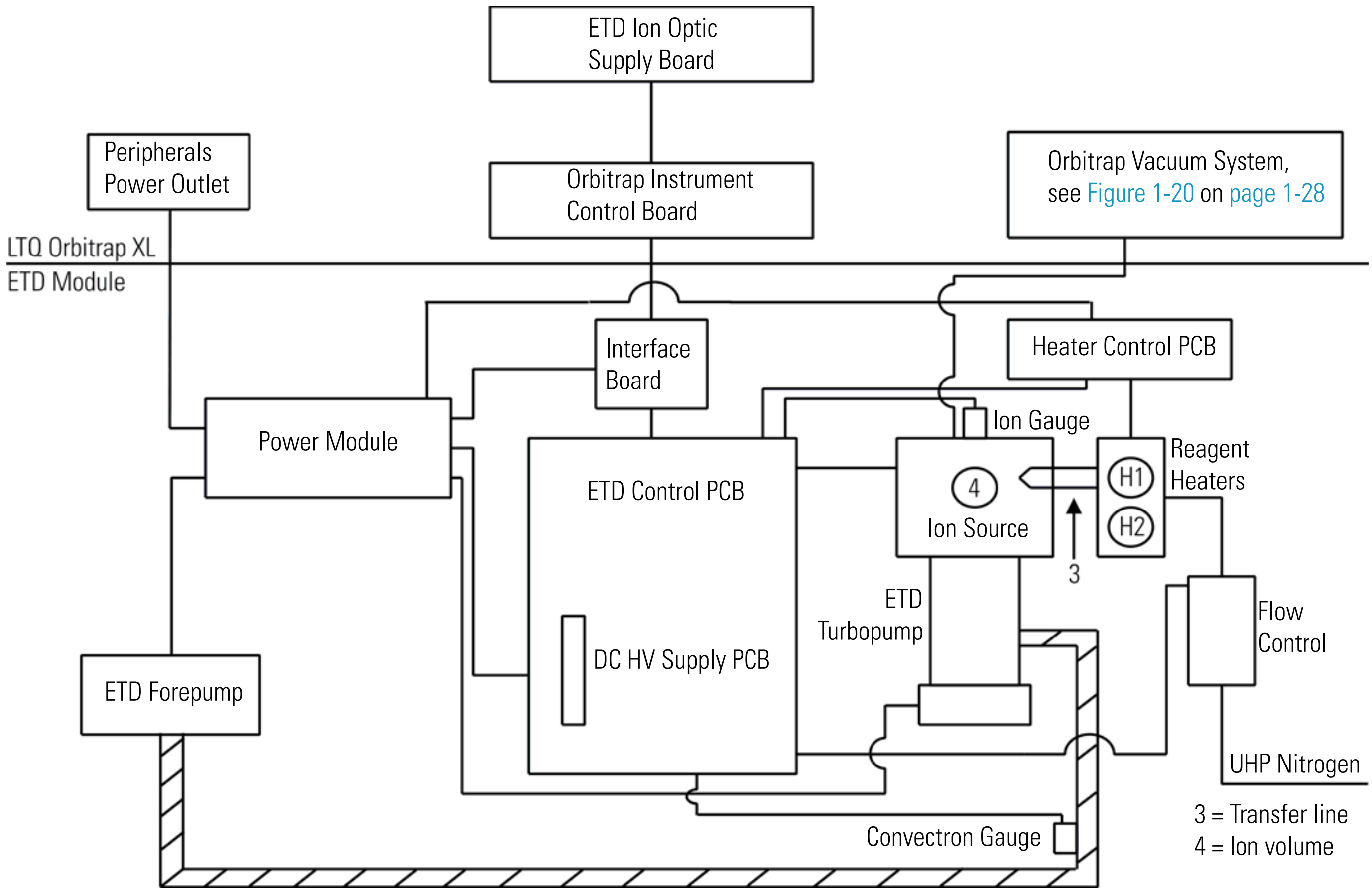


Figure 1-16. ETD Module functional block diagram

The following sections describe the major ETD Module components that are shown in Figure 1-15 on page 1-20 and Figure 1-16.

ETD Power Module

The ETD power module (item #1 in Figure 1-15) receives 220 V, 10 A, from the peripherals power outlet. See Figure 1-9 on page 1-11. 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 located on the ETD power module panel at the right side of the ETD Module. See Figure 1-5 on page 1-7 and Figure 1-17. Power In is connected to the peripherals power outlet. See Figure 1-9 on page 1-11. Forepump is a receptacle to power the ETD forepump (220 V AC, 5 A).

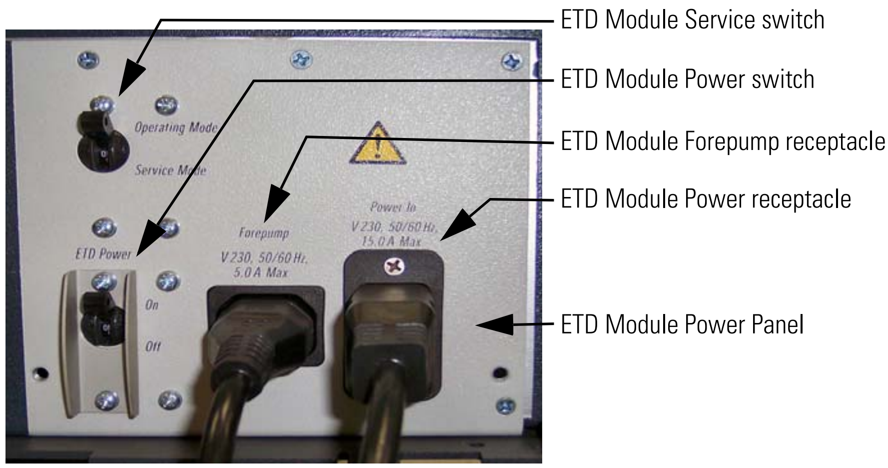


Figure 1-17. ETD Power Module panel

The ETD power module panel contains the main breaker and the service switch for the ETD Module. Use the main breaker to turn on or off all power to the ETD Module. The service switch turns On or Off power to all ETD Module components except the turbopump and forepump. During normal operation the ETD Power switch is left On and the service switch is left in the Operating Mode position.

ETD Module Interface Board

The ETD Module Interface board (item #2 in Figure 1-15) 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.

Note The ability to control the power to both components of the LTQ Orbitrap XL ETD 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 1-15) 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 1-15) is plugged in to the ETD Control PCB.

ETD Heater Control PCB

The ETD Module Heater Control PCB (item #6 in Figure 1-15) 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 1-16 on page 1-21, and items #9 and #10 in Figure 1-15), transfer line heater (#3 in Figure 1-15), and the restrictor oven heater (not shown in Figure 1-15). 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.

Nitrogen Flow Control for ETD

The reagent ion source in the ETD Module requires UHP nitrogen. The UHP nitrogen supply in the laboratory is connected to the UHP nitrogen port at rear side of the ETD Module. See Figure 1-29 on page 1-39. The ETD Module contains a digital flow control for UHP nitrogen (Figure 1-15 on page 1-20). This flow control is controlled by the ETD Control PCB (item #4 in Figure 1-15).

UHP nitrogen 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.

Note High-purity nitrogen is used to cool the reagent vials when the reagent ion source is turned off. ▲

Reagent Heaters

The reagent heaters (items #9 and #10 in Figure 1-15 on page 1-20, H1 andH2 in Figure 1-16 on page 1-21,) 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 (Figure 1-18).

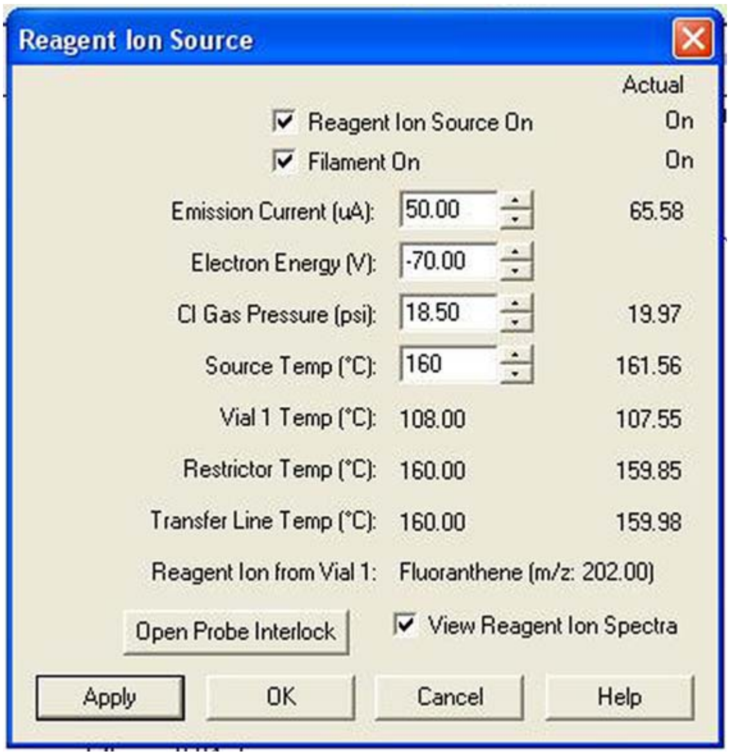


Figure 1-18. Reagent Ion Source dialog box

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

Note 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 topic "Turning Off the Reagent Ion Source: What to Expect" on page 2-14. ▲

Warning When the reagent ion source is in Off mode, the restrictor oven, the transfer line, and the ion source remain at 160 °C. ▲

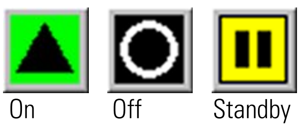
The nitrogen cooling gas turns off when the reagent heaters reach 70 °C. If it is necessary to install or replace the reagent vials, follow the procedure in topic "Changing the Reagent Vials" on page 3-48.

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

Warning Do not attempt 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 topic "Changing the Reagent Vials" on page 3-48 if it is necessary to install or replace the reagent vials. ▲

When the reagent heaters are in Standby mode, they are immediately turned on by selecting the Reagent Ion Source On check box (Figure 1-18). 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 delivered to the ion source.

Note 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 1-18 on page 1-24.)

- 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 1-15 on page 1-20 and inside of the vacuum manifold, see item #14 in Figure 1-15) 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 1-19. The ion source heater is controlled by the ETD Control PCB.

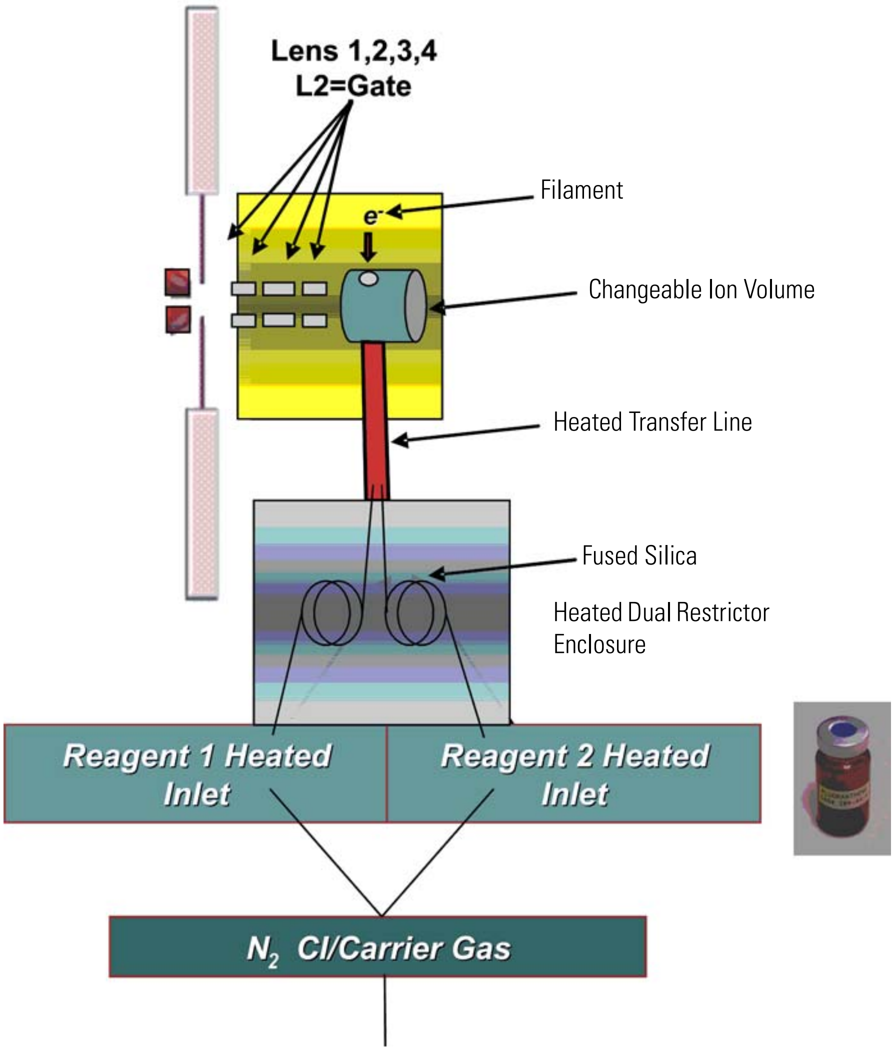


Figure 1-19. Reagent ion source schematics

The reagent ion source contains two reagent vials, CI/carrier gas (nitrogen) handling hardware and flow restrictors, the 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.

Vacuum System

Figure 1-20 shows a schematical overview of the Orbitrap vacuum system.

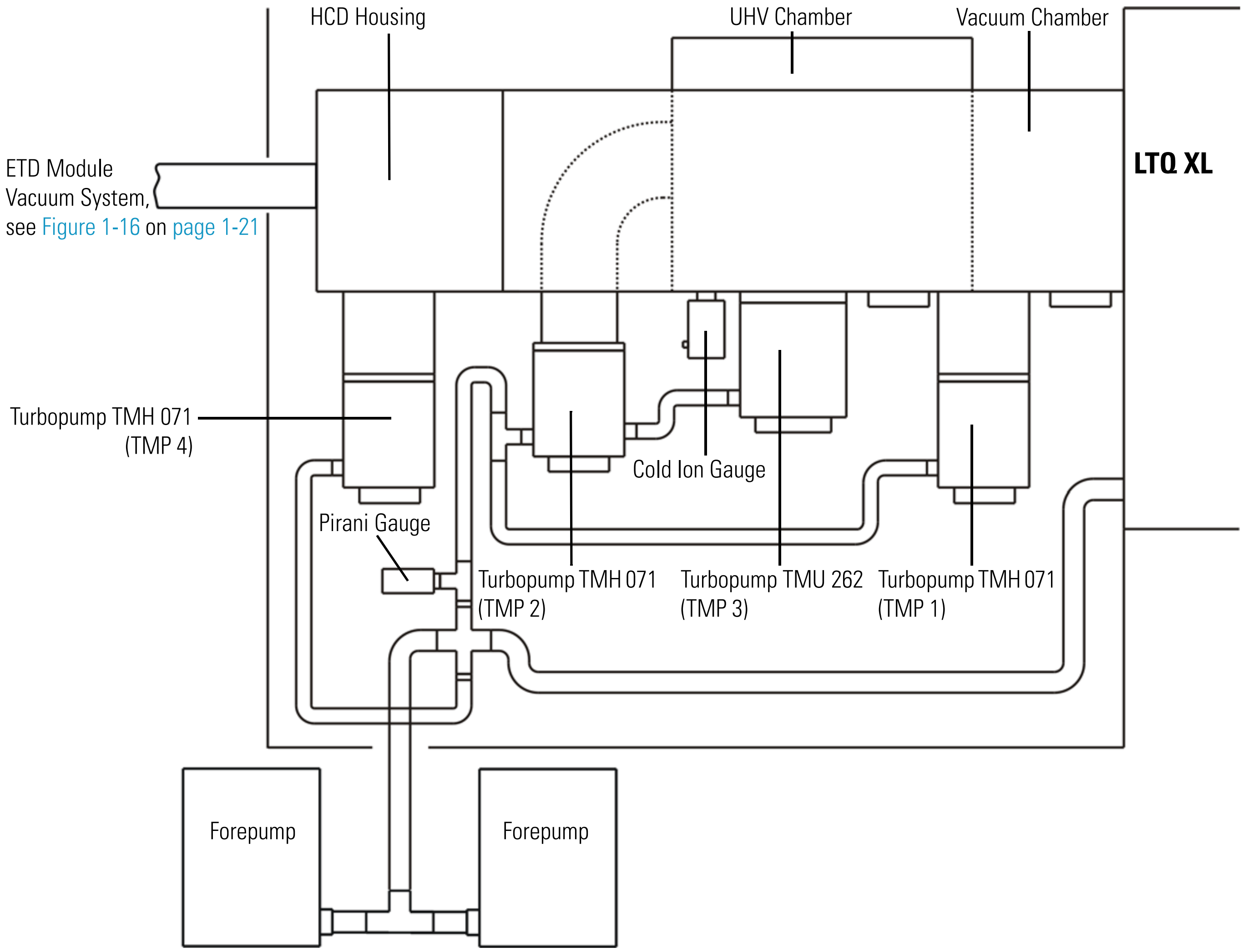


Figure 1-20. Schematical view of Orbitrap vacuum system (CLT compartment and Orbitrap chamber not shown)*

*For an abridged version of the parts list, see Table 4-7 on page 4-4.

The LTQ Orbitrap XL ETD 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 – turbopump TMH 071, TMP 1, manufacturer: Pfeiffer)
- **Ultra high vacuum chamber** (UHV chamber, pumped by a water-cooled 60 L/s turbopump TMH 071, TMP 2, manufacturer: Pfeiffer)

- **Orbitrap chamber** (pumped by a 210 L/s – for N_2 – water-cooled turbopump TMU 262, TMP 3, manufacturer: Pfeiffer)

- **HCD housing** (pumped by a water-cooled 60 L/s turbopump TMH 071, TMP 4, manufacturer: Pfeiffer)

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

Turbopumps

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 turbopump (**TMP 1**, see Figure 1-21). The rotary vane pumps of the linear trap (see below) provide the forevacuum for this pump. This chamber is bolted to a stainless steel welded UHV chamber housing the Orbitrap, lenses, and corresponding electrical connections.

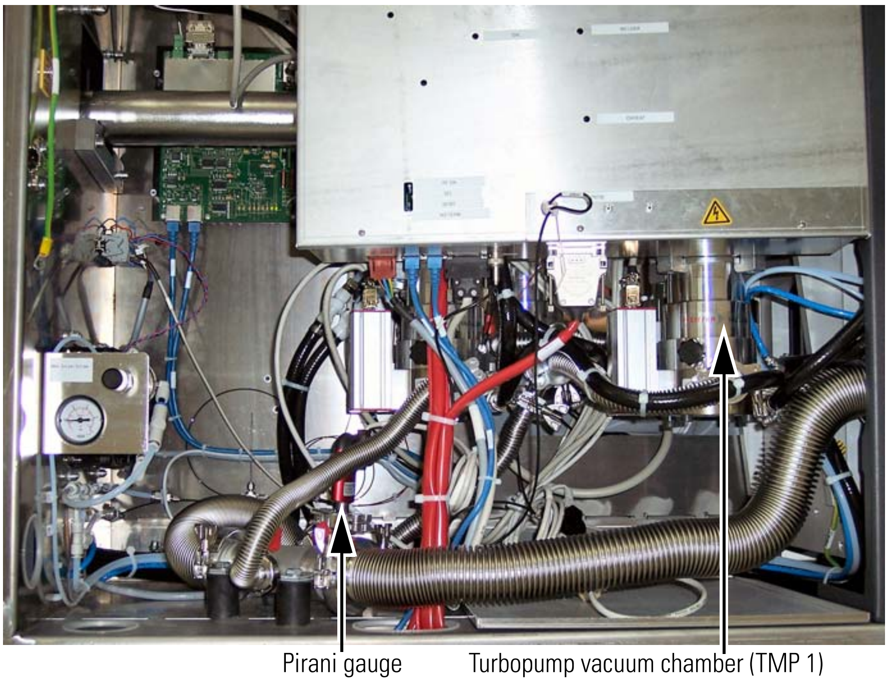


Figure 1-21. Vacuum components on the left instrument side

The UHV chamber is evacuated down to 10^{-8} mbar pressure range by a 60 L/s UHV turbopump (**TMP 2**, see Figure 1-22 on page 1-30).

The Orbitrap itself is separated from the UHV chamber by differential apertures and is evacuated down to 10^{-10} mbar by a 210 L/s turbopump (**TMP 3**, see Figure 1-22). All turbopumps are equipped with TC 100 control units (manufacturer: Pfeiffer).

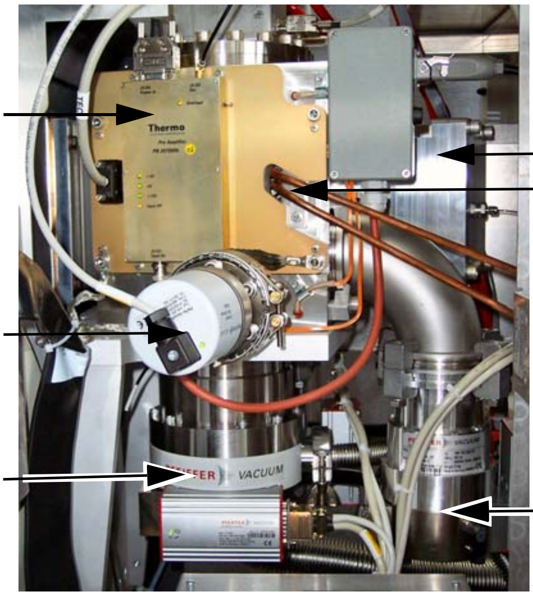


Figure 1-22. Vacuum components on the right instrument side

A tube, which contains the transfer multipole (flatapole), connects the HCD housing to the ETD Module. This part of the instrument is evacuated by a 60 L/s UHV turbopump (**TMP 4**, see Figure 1-23) at the bottom of the HCD housing.

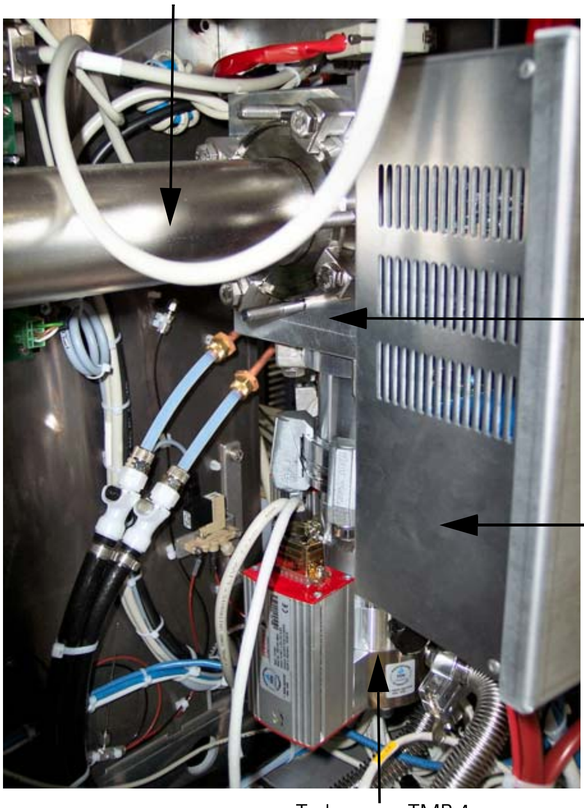


Figure 1-23. ETD mechanics

Linear Trap Turbopump

A separate turbopump 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 XL Hardware Manual*.

ETD Module Turbopump

A separate turbopump (Edwards EXT70H) provides the high vacuum for the ETD reagent ion source. See Figure 1-15 on page 1-20. It is backed up by a dedicated rotary vane pump at the bottom of the ETD Module. See Figure 1-25 on page 1-33. This turbopump contains no user-serviceable parts.

Forevacuum Pumps of the Linear Trap

The rotary vane pumps from the linear trap serve as forepumps for the three smaller turbopumps (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 are located on a small cart in the forepumps cabinet below the linear trap. See Figure 1-24.

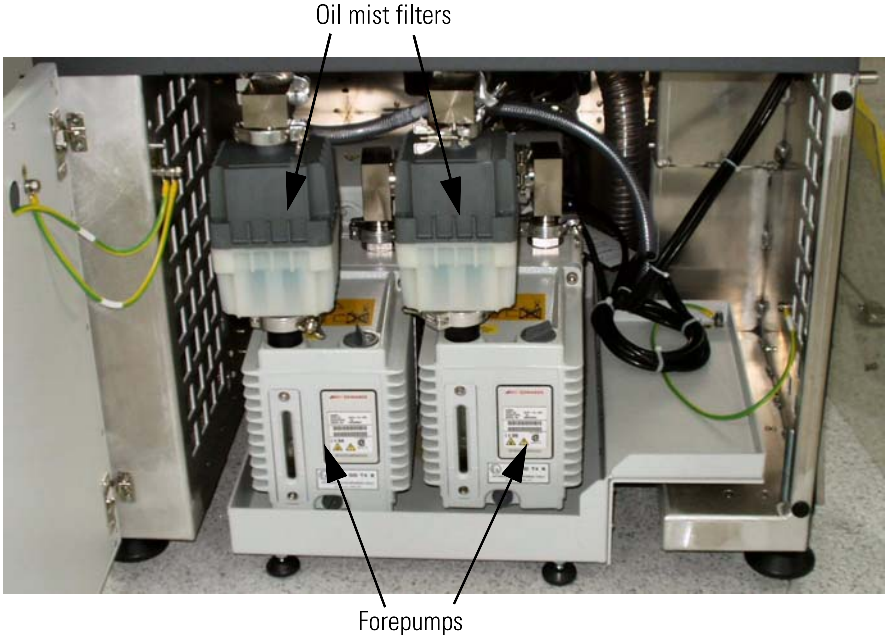


Figure 1-24. Forepumps cabinet

To minimize the ingress of pump oil into the exhaust system, the outlets of the forepumps are fitted to oil mist filters. See page 3-12 on instructions about returning the collected oil to the forepumps.

The forevacuum pumps (forepumps) of the linear trap are powered by the power panel of the linear ion trap.

Warning When analyzing hazardous materials, these may be present in the effluent of the forepumps! The connection to an adequate exhaust system is mandatory! ▲

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.

Forevacuum Pump of the ETD Module

A rotary vane pump (BOC Edwards RV 3) provides the forevacuum for the ETD turbopump. It is located in a cabinet at the bottom of the ETD Module. The forepump is equipped with an oil mist filter and stands on a drip pan. See Figure 1-25 on page 1-33.

An exhaust hose connects the forepump to the exhaust system in the laboratory. A forevacuum tube connects the ETD forepump to the ETD turbopump. The forepump electrical cord is plugged into the Forepump receptacle on the ETD Module power panel. See Figure 1-17 on page 1-22.

For maintenance instructions for the ETD forepump, see topic "Maintenance of the ETD Forepump" on page 3-5 and the manual that came with the forepump.

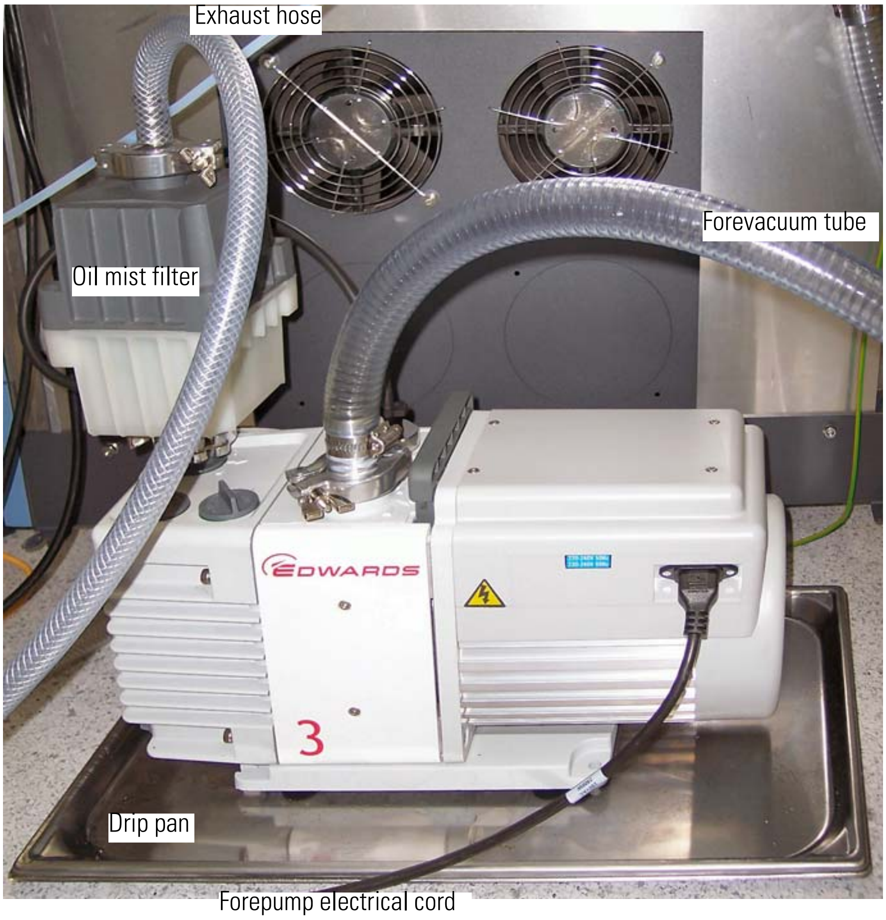


Figure 1-25. Forepump for ETD Module

Vacuum System Controls

The power distribution board controls all turbopumps via voltage levels. Refer to topic "Power Distribution Board" on page 1-52. An interface for RS485 data via the instrument control board connects the turbopumps with the linear ion trap. (Refer to topic "Instrument Control Board" on page 1-50.) The turbopump of the linear ion trap and the ETD turbopump have individual controllers.

Vacuum Gauges

The vacuum is monitored by several vacuum gauges:

- The forevacuum of the LTQ Orbitrap XL ETD is monitored by an Active Pirani gauge (TPR 280, manufacturer: Pfeiffer) connected to the LTQ Orbitrap XL ETD forevacuum line. See Figure 1-21 on page 1-29.

- The high vacuum of the LTQ Orbitrap XL ETD is monitored by a Cold Ion Gauge (IKR 270, manufacturer: Pfeiffer) connected to the UHV chamber. See Figure 1-22 on page 1-30. Because the gauge would be contaminated at higher pressures, it is turned 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 XL Hardware Manual* for more information.

- Two dedicated vacuum gauges monitor the vacuum in the ETD Module. A Convectron gauge (see Figure 1-15 on page 1-20 and Figure 1-16 on page 1-21)) monitors the pressure in the ETD forevacuum line and an ion gauge (see Figure 1-15) monitors the pressure in the reagent ion source. Table 1-3 shows typical pressure readings in the ETD Module.

Table 1-3. Typical pressure readings in the ETD Module

Conditions	Convection Gauge Reading (foreline, capillary skimmer region)	Ion Gauge Reading (analyzer region)
CI gas pressure set to 20 psi	0.1–0.01 Torr	$20–35\times10^{-5}$ Torr

The vacuum gauges of the LTQ Orbitrap XL ETD are connected to the power distribution board that directly responds to the pressure values. (Refer to the topic "Power Distribution Board" on page 1-52.) The analog values are digitized by the instrument control board. (Refer to the topic "Instrument Control Board" on page 1-50.) 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 Pumps & Electronics switch is switched On, the pumps of the linear ion trap and the LTQ Orbitrap XL ETD are run up. The Pirani gauge (see above) controls the LTQ Orbitrap XL ETD 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 turbopumps (e.g. 80% after 15 min.).

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 region.

Vacuum Failure

In case the pressure in the LTQ Orbitrap XL ETD 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. (Refer to the topic “Power Distribution Board” on page 1-52.) It can be reset by switching the main power switch off and on. (Refer to the topic “Main Power Switch” on page 1-10.)

Upon venting, the vent valves of the turbopumps on the Orbitrap detector stay closed. Only the vent valve of the linear ion trap is used. (Refer to the topic “Vent Valve of the Linear Ion Trap” on page 1-38.)

Vacuum System Heating during a System Bakeout

After the system has been open to the atmosphere (e.g. 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. Refer to the topic “Baking Out the System” on page 3-4.

Gas Supply

This section describes the gas supplies for the mass analyzers and the reagent ion source of the LTQ Orbitrap XL ETD.

Gas Supply for the Mass Analyzers

Figure 1-26 shows a schematical view of the gas supply for the instrument.

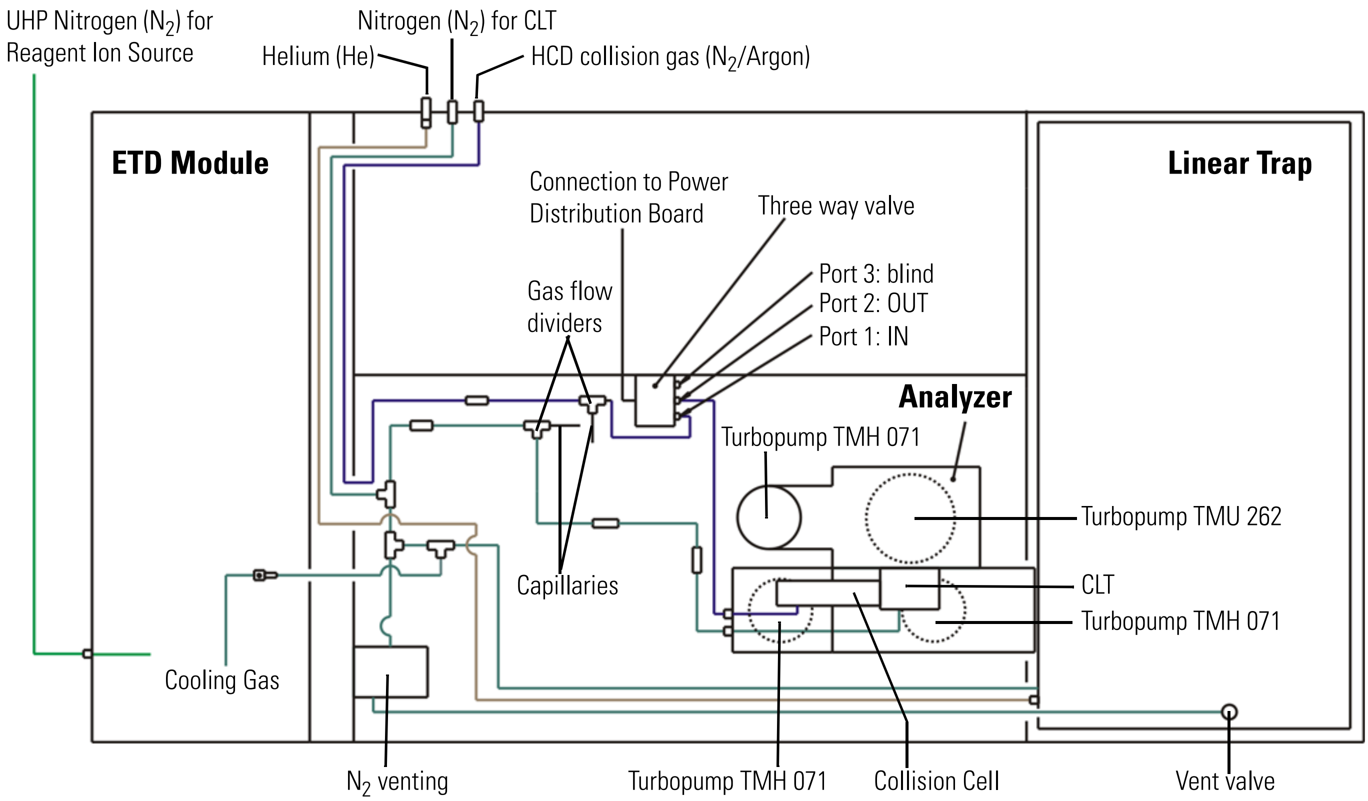


Figure 1-26. Schematical view of the gas supply*

*For parts lists of the gas supply, refer to Table 4-10 on page 4-5 and to Table 4-30 on page 4-14.

The mass analyzers use at least two gases for operation:

- The linear trap requires high-purity (99%) nitrogen for the API sheath gas and auxiliary/sweep gas. The Orbitrap uses high-purity nitrogen as collision gas (bath gas) for the curved linear trap and the HCD collision octapole. The ETD system uses high-purity nitrogen for cooling the reagent vials when the reagent ion source is turned off.

Note In addition to high-purity nitrogen, the LTQ Orbitrap XL ETD requires ultra-high purity nitrogen. See topic "Gas Supply of the Reagent Ion Source" on page 1-39 for details. ▲

- The linear trap requires ultra-high purity (99.999%) helium for the collision gas.
- In case argon is used as HCD collision gas, it should be of high purity (99.99%).

The laboratory gas supply is connected to the inlets at the right side of the instrument. See Figure 1-9 on page 1-11. Within the instrument, the helium gas is led from the helium port through a stainless steel capillary to the right rear side of the linear trap. High purity nitrogen gas and HCD collision gas are both led via Teflon tubing to the right side of the LTQ Orbitrap XL ETD.

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 below for further information.) Another part of the nitrogen flow is directed through Teflon tubing to the vacuum chamber of the Orbitrap. 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 turned off.

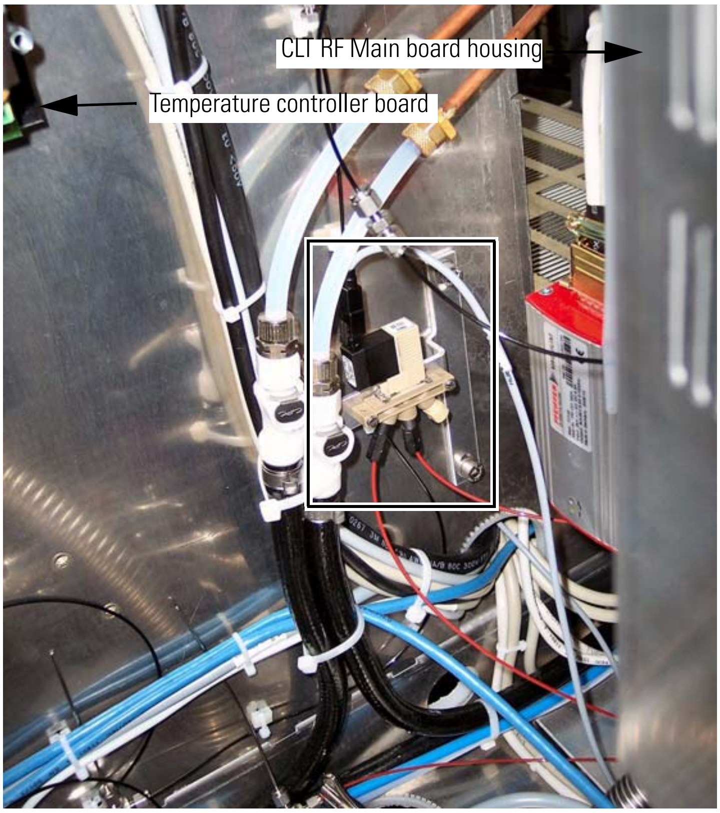


Figure 1-27. Valve for HCD collision gas

Nitrogen gas pressure to the C-Trap is kept constant by using an “open-split” interface (gas flow divider, see Figure 1-28 on page 1-38). It contains a capillary line from the nitrogen line of the instrument to atmosphere (flow rate: ~20 mL/min), with another capillary leading from the point of atmospheric pressure into the C-Trap (flow rate: ~0.2 mL/min). For the nitrogen gas to the C-Trap, *black* PEEKSil™ tubing is used (75 µm ID silica capillary in 1/16” PEEK tubing).

The HCD collision gas is also led to a gas flow divider. Part of the gas is led through a capillary line to the atmosphere (flow rate: ~20 mL/min). The other part of the gas (flow rate: ~0.5 mL/min) enters the IN port of a three way valve. The gas leaves the valve through the OUT port and is led to the collision octapole next to the curved linear trap.[1] For the HCD collision gas, *red* PEEKSil™ tubing is used (100 µm ID silica capillary in 1/16” PEEK tubing).

The HCD collision gas valve is located at the left instrument side next to the temperature controller board. See Figure 1-27 on page 1-37. It is switched by the software via the power distribution board. (See page 1-52.)

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 XL Hardware Manual* contains further information about the vent valve.

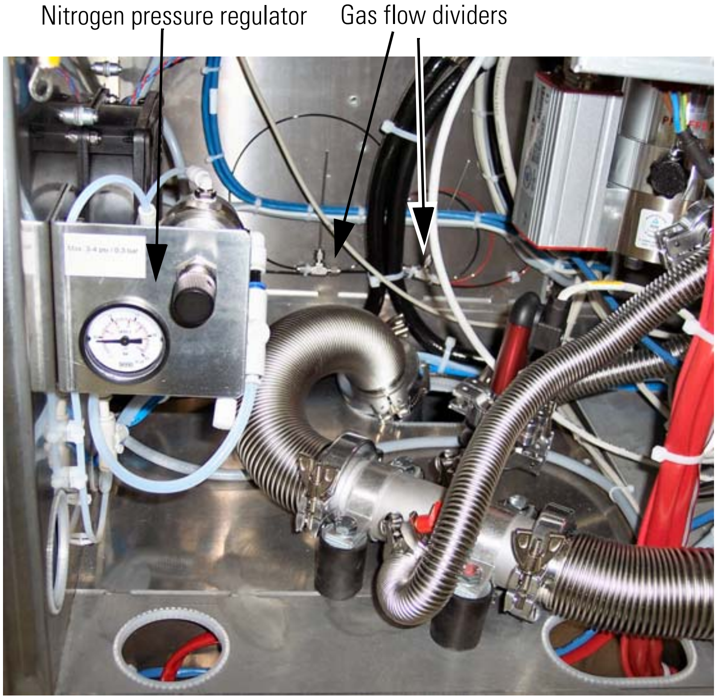


Figure 1-28. Nitrogen pressure regulator and gas flow dividers

[1]The third port of the valve is closed.

The instrument is vented with high purity nitrogen from the same tubing that supplies the LTQ XL sheath gas. See Figure 1-26 on page 1-36. The vent valve of the LTQ XL is attached to a pressure regulator that is set to a venting pressure of 3–4 psi. The pressure regulator is located at the left side of the LTQ Orbitrap XL ETD. See Figure 1-28.

Gas Supply of the Reagent Ion Source

In addition to high purity nitrogen for cooling, the reagent ion source of the LTQ Orbitrap XL ETD uses ultra high purity (UHP, 99.995%) nitrogen gas as carrier gas and chemical ionization (CI) vehicle. The UHP nitrogen supply of the laboratory is connected to the inlet port at the rear side of the instrument. See Figure 1-29.

Figure 1-29. UHP nitrogen port at the ETD Module

Cooling Water Circuit

Figure 1-30 on page 1-40 shows a schematical view of the cooling water circuit in the LTQ Orbitrap XL ETD. Cooling water at a temperature of 20 °C enters and leaves the instrument at the bottom of the right side. See Figure 1-9 on page 1-11. First, the fresh water passes through the turbopumps 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. Before it leaves the instrument, the water passes through the other Peltier element at the back of the central electrode power supply board.

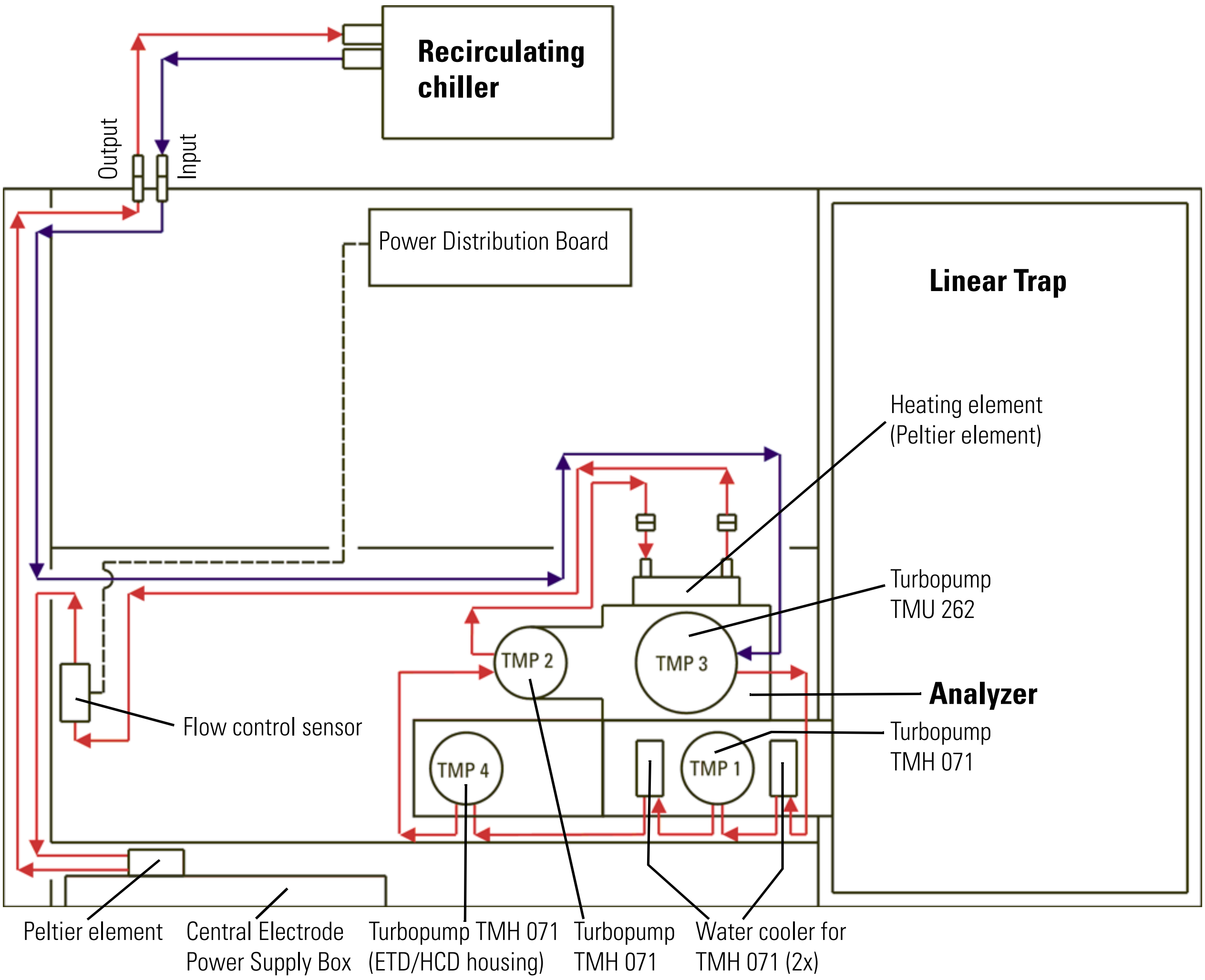


Figure 1-30. Schematical view of cooling water circuit*

*For a parts list of the cooling water circuit, refer to Table 4-12 on page 4-6.

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.

Recirculating Chiller

A recirculating chiller (NESLAB ThermoFlex™ 900) is delivered with the instrument, making the LTQ Orbitrap XL ETD independent from any cooling water supply. A wall receptacle provides the electric power for the chiller. Two water hoses (black), internal diameter 9 mm, wall thickness 3 mm, length approx. 3 m (~10 ft) are delivered with the instrument.

For instruction about performing maintenance for the chiller, see topic "Maintenance of the Recirculating Chiller" on page 3-61. See also the manufacturer's manual for the chiller.

Properties of Cooling Water

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.

The cooling water should meet the following requirements:

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

Warning **Danger of Burns!**
If the water circuit fails, all parts of the water distribution unit may be considerably heated up. Do not touch the parts!
Before disconnecting the cooling water hoses, make sure the cooling water has cooled down! ▲

Printed Circuit Boards

The LTQ Orbitrap XL ETD 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 mass analyzer.

The following pages contain a short overview of the electronic boards in the MS portion of the LTQ Orbitrap XL ETD. 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 topic "ETD Module" on page 1-19.

The electronics of the LTQ Orbitrap XL ETD contains complicated and numerous circuits. Therefore, only qualified and skilled electronics engineers should perform servicing.

A Thermo Fisher Scientific 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.

Warning **Parts of the printed circuit boards are at high voltage.** Opening the electronics cabinet is only allowed for maintenance purposes by qualified personal. ▲

Note Many of the electronic components can be tested by the LTQ Orbitrap XL ETD diagnostics, which is accessible from the Tune Plus window. ▲

Linear Ion Trap Electronics

The linear ion trap is connected to the LTQ Orbitrap XL ETD main power switch. The linear ion trap has a sheet metal back cover. Figure 1-31 shows the electronic connections at the rear side of the linear trap.

Figure 1-31. Electronic connections to linear trap (covers removed)

The linear ion trap electronics has two connections with the LTQ Orbitrap XL ETD electronics:

- Data communication with the internal computer of the LTQ Orbitrap XL ETD. Refer to the topic "Electronic Boards at the Right Side of the Instrument" on page 1-44.

- Signal communication (SPI bus) with supply information for the instrument control board. Refer to the topic "Instrument Control Board" on page 1-50.

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

Electronic Boards at the Right Side of the Instrument

Figure 1-32 shows the parts of the instrument when the right side panel is opened. A transparent cover protects the lower part.

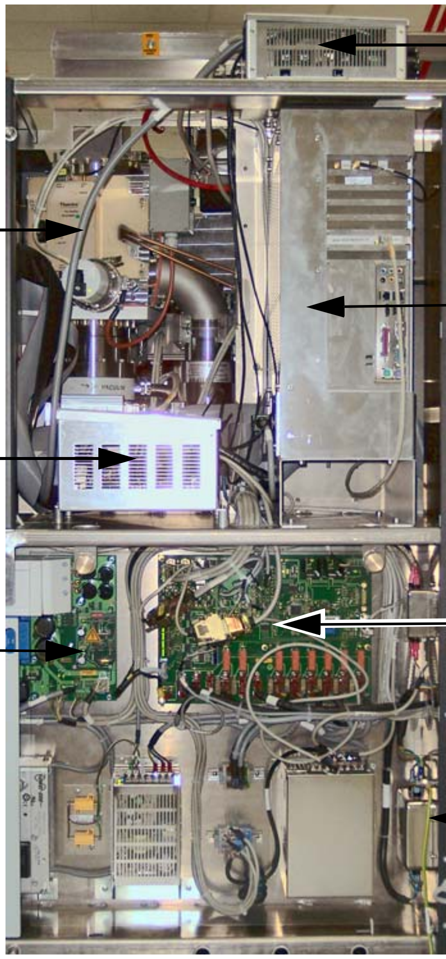


Figure 1-32. Electronic boards on the right side of the instrument

The side panel is connected to the instrument frame by two green/yellow ground wires. See bottom of Figure 1-32. 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 (P/N 210 8920)[1] is mounted on top of the data acquisition unit. See Figure 1-33. It 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.

[1]Part number of complete unit.

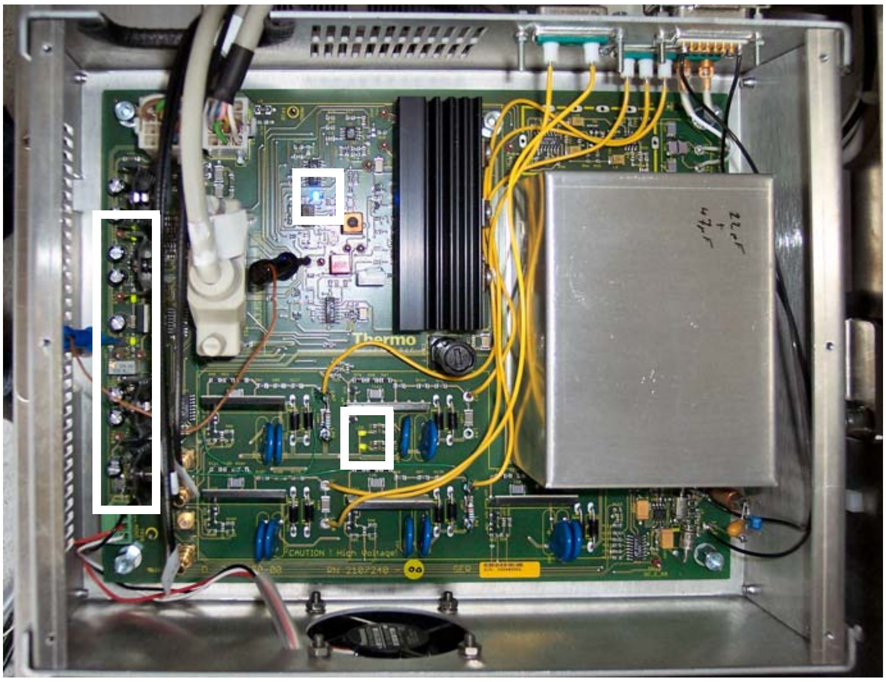


Figure 1-33. ETD Ion Optic Supply board

The diagnostic LEDs on the ETD ion optic supply board are listed in Table 1-4 on page 1-45. The positions of the diagnostic LEDs on the board are indicated by white rectangles in Figure 1-34.

Table 1-4. 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

Figure 1-34 shows the preamplifier (P/N 207 8900)[1]. The preamplifier is located in a housing next to the Cold Ion Gauge.

Figure 1-34. Preamplifier board

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 1-5 on page 1-47. The positions of the diagnostic LEDs on the board are indicated by white rectangles in Figure 1-34.

[1] Part number of complete unit.

Table 1-5. 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 1-35 shows the components of the data acquisition unit (P/N 206 4132). The unit is mounted in a housing located at the right side of the instrument.

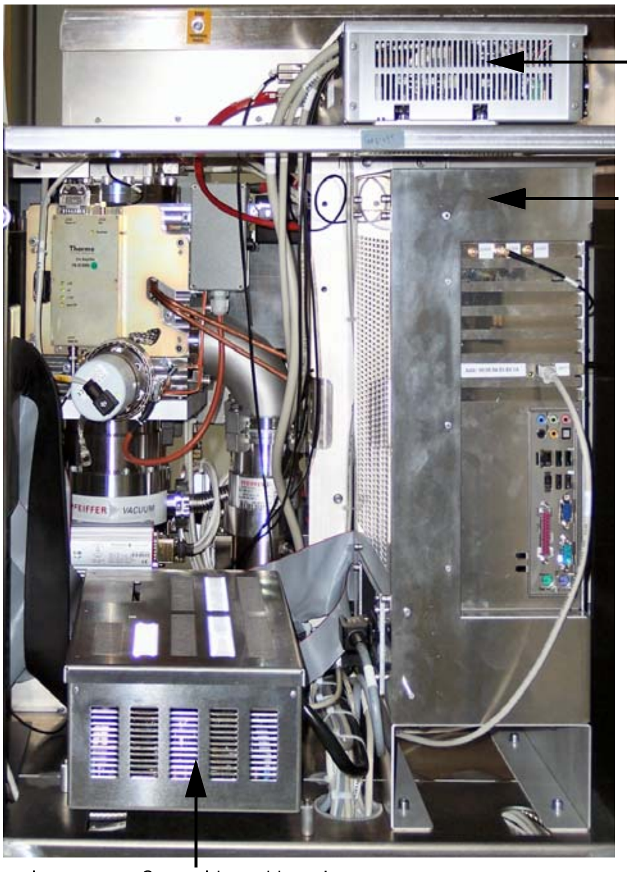


Figure 1-35. Data Acquisition unit

The internal computer (P/N 207 6470) 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 1-36 shows the data acquisition digital PCI board (P/N 206 0501). It is an add-on board to the internal computer. (See Figure 1-35 on page 1-47.)

Figure 1-36. 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 is 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 ion trap and the internal computer of the LTQ Orbitrap XL ETD system, but also between the ion trap and the data system computer. For further information about the data system, refer to the *LTQ XL Hardware Manual*.

The diagnostic LEDs listed in Table 1-6 on page 1-49 show the status of the board. The position of the LEDs on the board is indicated by a white rectangle in Figure 1-36.

Table 1-6. 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 1-37 shows the data acquisition analog board (P/N 206 4150).

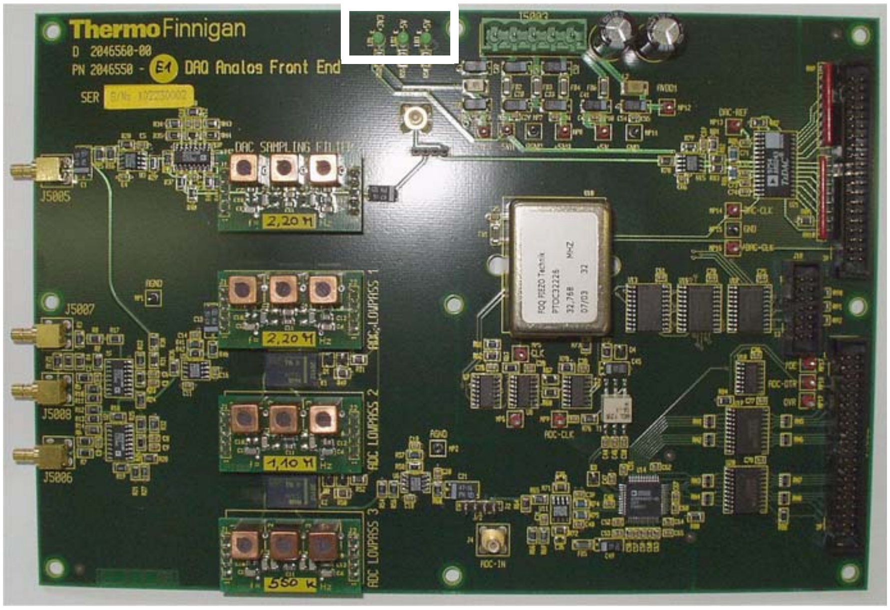


Figure 1-37. Data Acquisition Analog board

This board is an add-on board to the mainboard of the internal computer. See Figure 1-35 on page 1-47. It is used to convert analog to digital signals for Orbitrap 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.

The diagnostic LEDs listed in Table 1-7 on page 1-50 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 1-37.

Table 1-7. 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 (P/N 206 1440) 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 1-35 on page 1-47.

The diagnostic LEDs listed in Table 1-8 show the status of the voltages applied to the board.

Table 1-8. 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 1-38 shows the instrument control board (P/N 205 4221). The instrument control board is located in a housing next to the internal computer. It is connected to the LTQ Orbitrap XL ETD main power.

The instrument control board is used to interface the LTQ XL control electronics to the Orbitrap control electronics. Three signal lines are passed from the LTQ XL: 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 1-52.) Turbopumps (Refer to the topic “Vacuum System” on page 1-28.) are attached to a serial port connector and this is connected via the signal lines to the linear ion trap.

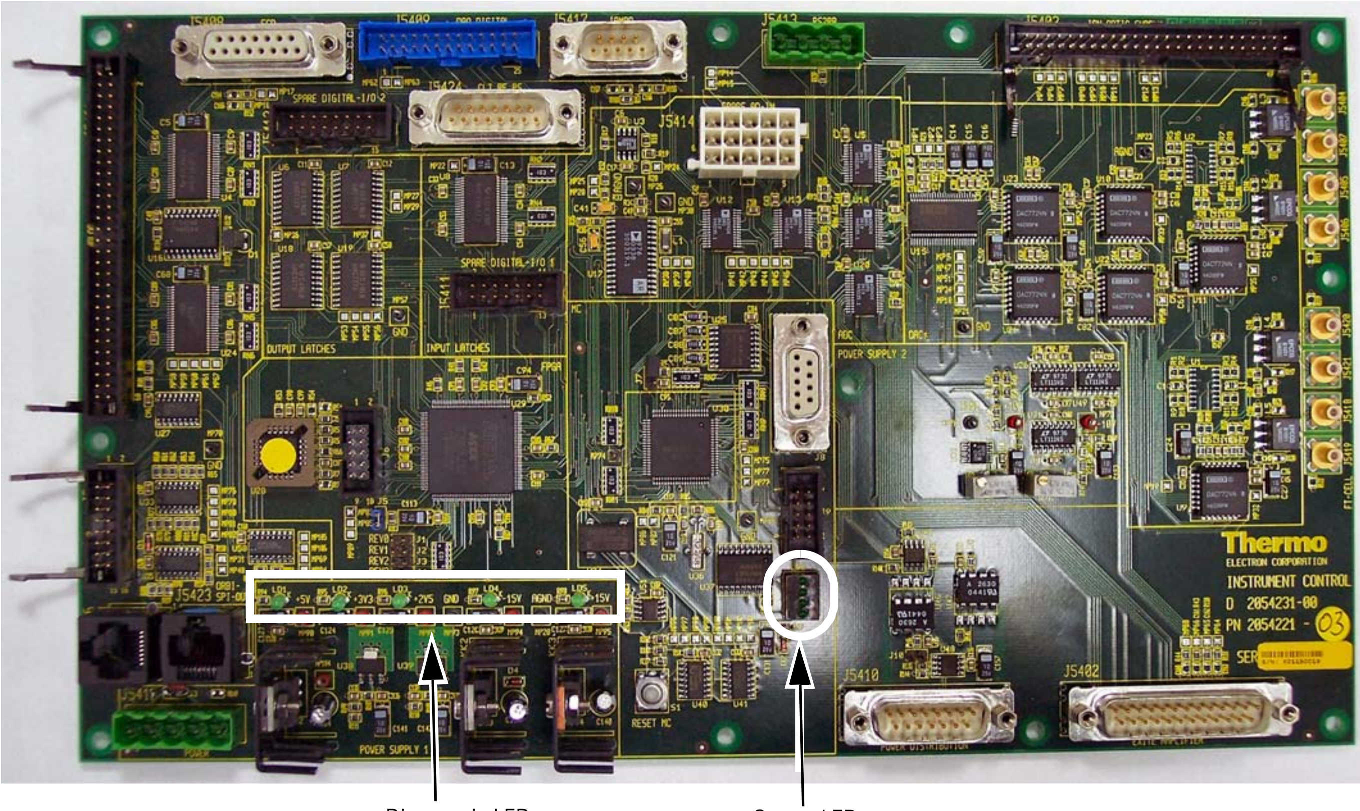


Figure 1-38. Instrument Control board

The diagnostic LEDs listed in Table 1-9 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 1-38.

Table 1-9. 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 1-10 on page 1-52. The position of the status LEDs on the board is indicated by a white oval in Figure 1-38 on page 1-51.

Table 1-10. 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 LTQ XL SPI bus enabled	On
6.4	Orbitrap SPI bus enabled	On Flashing on error

Power Distribution Board

Figure 1-39 on page 1-52 shows the power distribution board (P/N 206 2130)[1]. It is located at the bottom of the right side of the instrument.

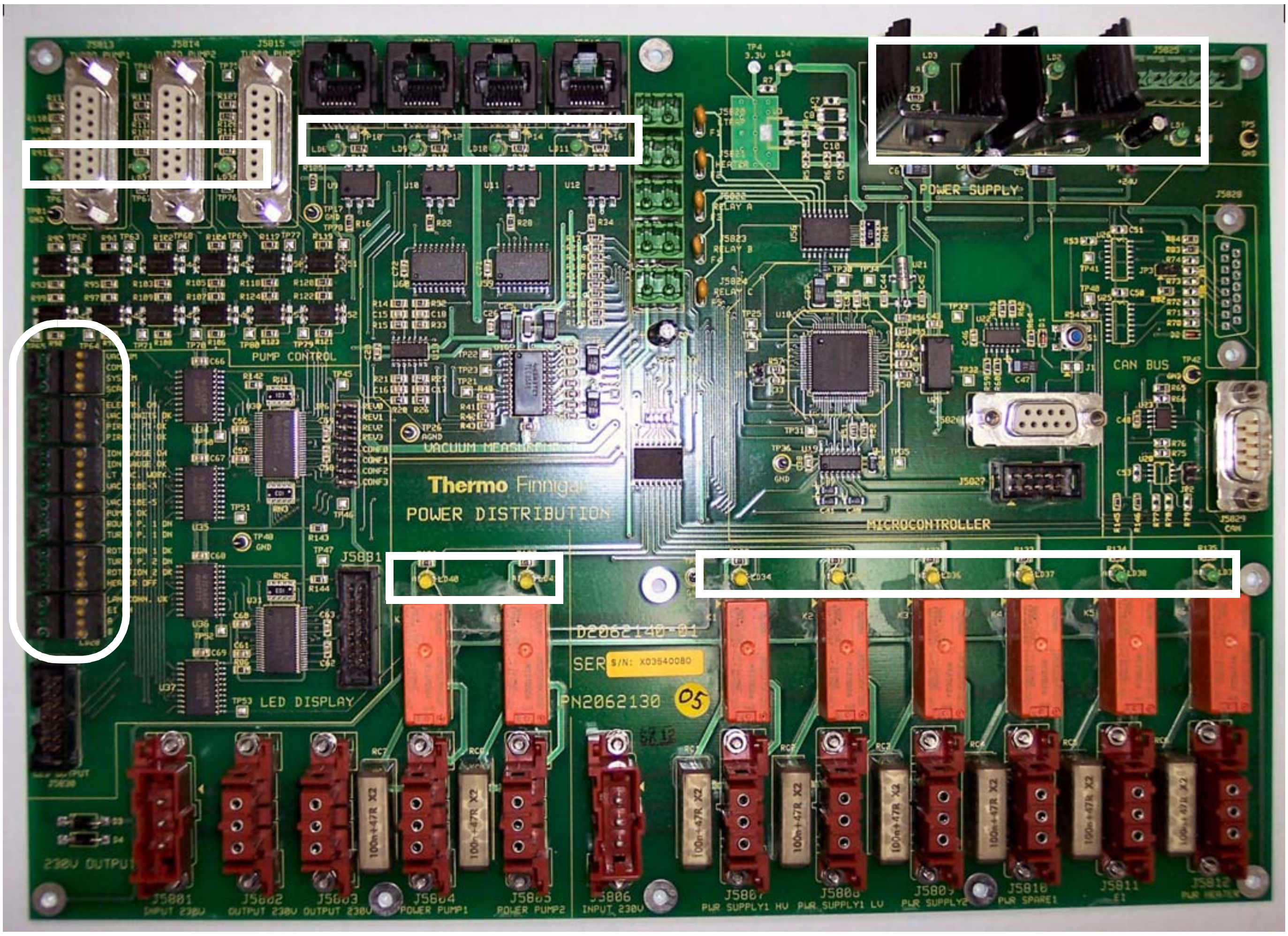


Figure 1-39. Power Distribution board

[1]Part number of complete unit.

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. The board also switches the valve that controls the flow of the HCD collision gas.

The power distribution board indicates all system states and error messages by status LEDs (see Table 1-11 on page 1-54) 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 1-39 on page 1-52.

The system status LEDs on the front side of the instrument (See Figure 1-4 on page 1-6.) 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). (Refer to topic "Instrument Control Board" on page 1-50.)

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 1-39 on page 1-52.

Table 1-11. 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 OK	No function, at present	
Pirani LT OK	Pirani LTQ XL failure	Control signal < 0.5 V
Ion Gauge On	Penning LTQ Orbitrap XL ETD Off	Forevacuum > 10^{-2} mbar
Ion Gauge OK	Penning LTQ Orbitrap XL ETD failure	Control signal < 0.5 V
LT Vacuum Work	LTQ XL vacuum failure	Vacuum forepump LTQ XL >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	Turbopump #1 failure	Turbopump defective/error*
Rotation 1 OK	Turbopump #1 failure	80% rotation speed of turbopump not reached
Turbo P. 2 On	Turbopump #2 failure	Turbopump defective/error*
Rotation 2 OK	Turbopump #2 failure	80% rotation speed of turbopump 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 occured
B		Micro controller idle

*An error of turbopump 3 is indicated by an LED directly located on the pump controller. An error of turbopump 4 is indicated in the software.

Depending on user actions, the power distribution is switched to various working modes by the hardware. See Table 1-12.

Table 1-12. 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 • LTQ XL (has a separate Service switch)

Table 1-13 shows the possible operating states of the power distribution.

Table 1-13. 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 LTQ Orbitrap XL ETD forevacuum pumps: 10^{-0} mbar after 30 s.	If not ok: switch off system and light error LED*; power distribution remains switched on
4.	After the system has started, the Pirani gauge returns a vacuum < 10^{-2} mbar and both turbopumps reach 80% rotation speed	Switch on Penning gauge
5.	Vacuum and 80% rotation speed of turbopumps 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

Table 1-13. Operating states of the Power Distribution board, continued

	Action	Consequences
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 LTQ Orbitrap XL ETD >10^{-1} mbar • Penning gauge LTQ Orbitrap XL ETD >10^{-3} mbar • Pirani gauge LT 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 turbopump falls below 80%	Shut down system (see 7.); light LED* of corresponding pump.
9.	Service switch linear ion trap off	Linear ion trap electronics switched off, pumps keep on running; LTQ Orbitrap XL ETD without data link, keeps on running
10.	FT Electronics switch LTQ Orbitrap XL ETD off	LTQ Orbitrap XL ETD electronics switched off, pumps keep on running; LTQ Orbitrap XL ETD without data link, keeps on running
11.	Failure of linear ion trap or LTQ Orbitrap XL ETD (e.g. 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.

* After the shutdown, the LED flashes that represents the reason for the shutdown.

Power Supply 1 Board

Figure 1-40 on page 1-57 shows the power supply 1 board (P/N 205 5810). This board is located next to the power distribution board. It provides the power for the ion optic supply board (Refer to topic "Ion Optic Supply Board" on page 1-59.) and the instrument control board. (Refer to topic "Instrument Control Board" on page 1-50.)

Figure 1-40. Power Supply 1 board

Warning Parts of the power supply 1 board are at high voltage. ▲

The diagnostic LEDs listed in Table 1-14 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 1-40.

Table 1-14. 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 1-41 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 control.

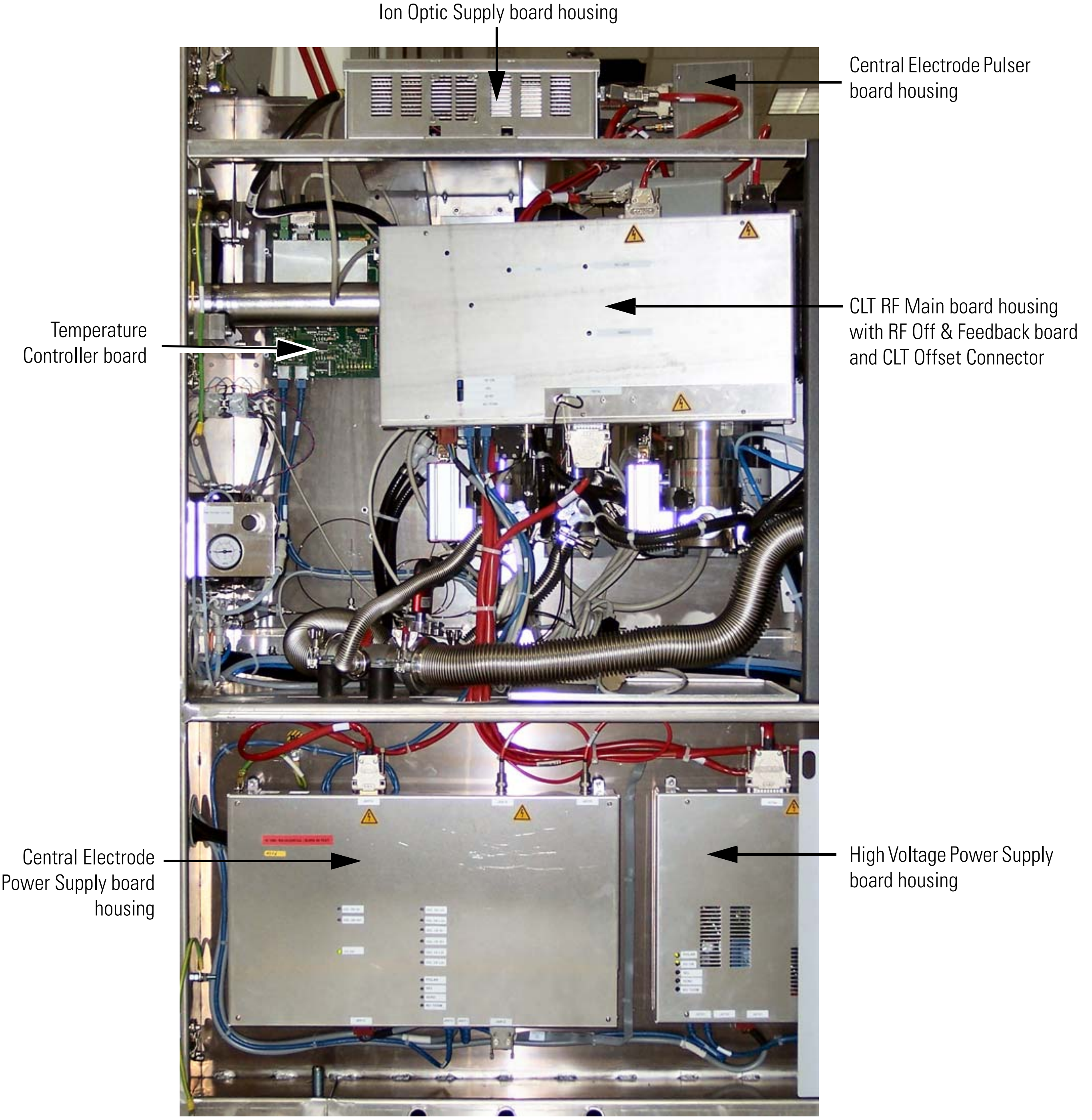


Figure 1-41. Electronic boards on the left side of the instrument

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

Ion Optic Supply Board

Figure 1-42 shows the ion optic supply board (P/N 209 9810)[1]. The board is located 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 LTQ Orbitrap XL ETD. 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. See topic "Orbitrap Analyzer" on page 1-13 for further information. Furthermore, the board provides the voltages for the HCD collision cell. See page 1-18.

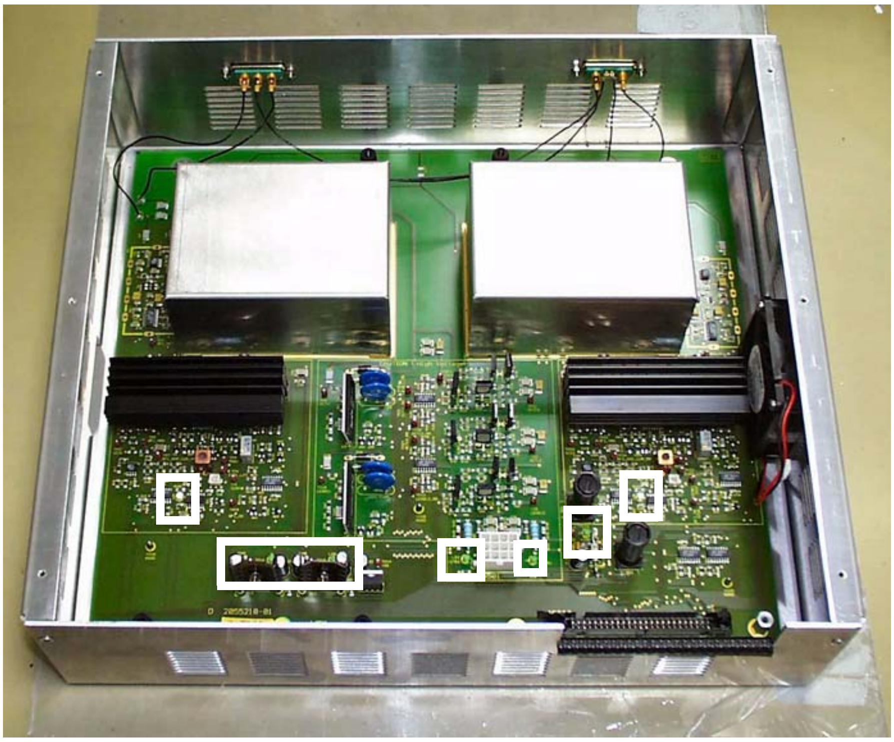


Figure 1-42. Ion Optic Supply board

The diagnostic LEDs listed in Table 1-15 on page 1-60 show the status of applied voltages to the board. The position of the LEDs on the board is indicated by white rectangles in Figure 1-42.

Warning Parts of the board are at high voltage. ▲

[1]Part number of complete unit.

Table 1-15. 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 (P/N 207 9640)[1] is located in a housing that is mounted to the flange of the UHV chamber.

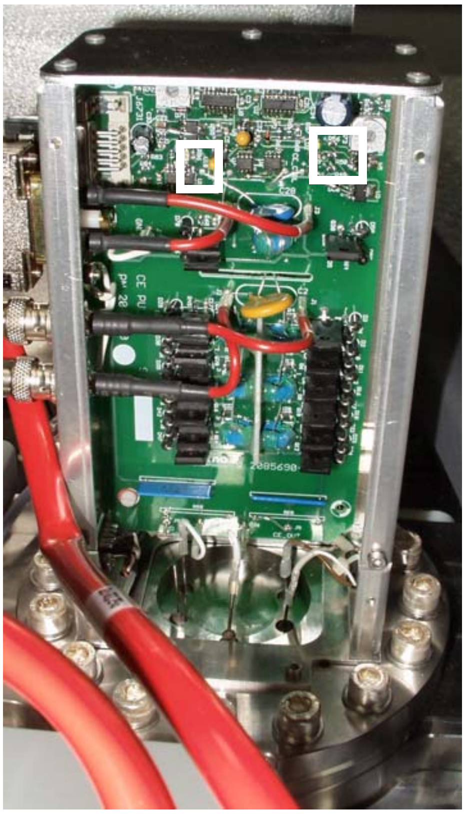


Figure 1-43. Central Electrode Pulser board

[1]Part number of complete unit.

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

The diagnostic LEDs listed in Table 1-16 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 1-43 on page 1-60.

Table 1-16. 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	24V Power Supply is OK	On

Temperature Controller Board

The temperature controller board (P/N 207 8930) is located on the top left side of the instrument, next to the CLT RF main board. See Figure 1-41 on page 1-58. 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.

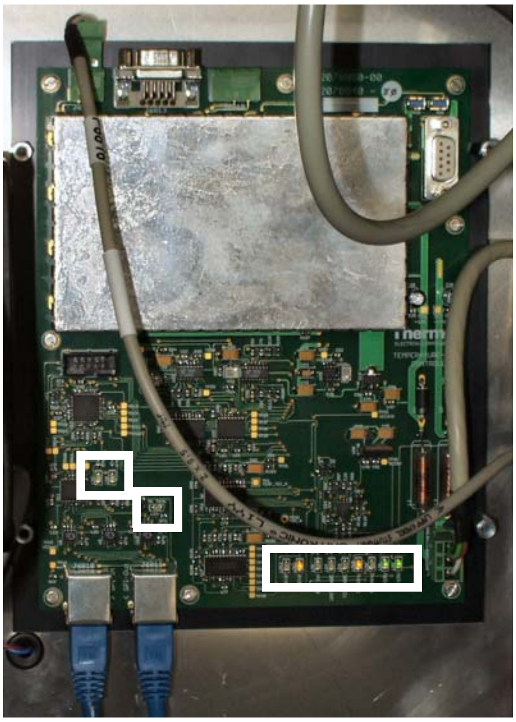


Figure 1-44. Temperature Controller board

The diagnostic LEDs listed in Table 1-17 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 1-44.

Table 1-17. 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 (P/N 207 9581) 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 (P/N 207 9591) is located in a housing in the center of the left side of the instrument. See Figure 1-41 on page 1-58. 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 topic “Orbitrap Analyzer” on page 1-13 for further information. The board communicates with the instrument control board via an SPI bus.

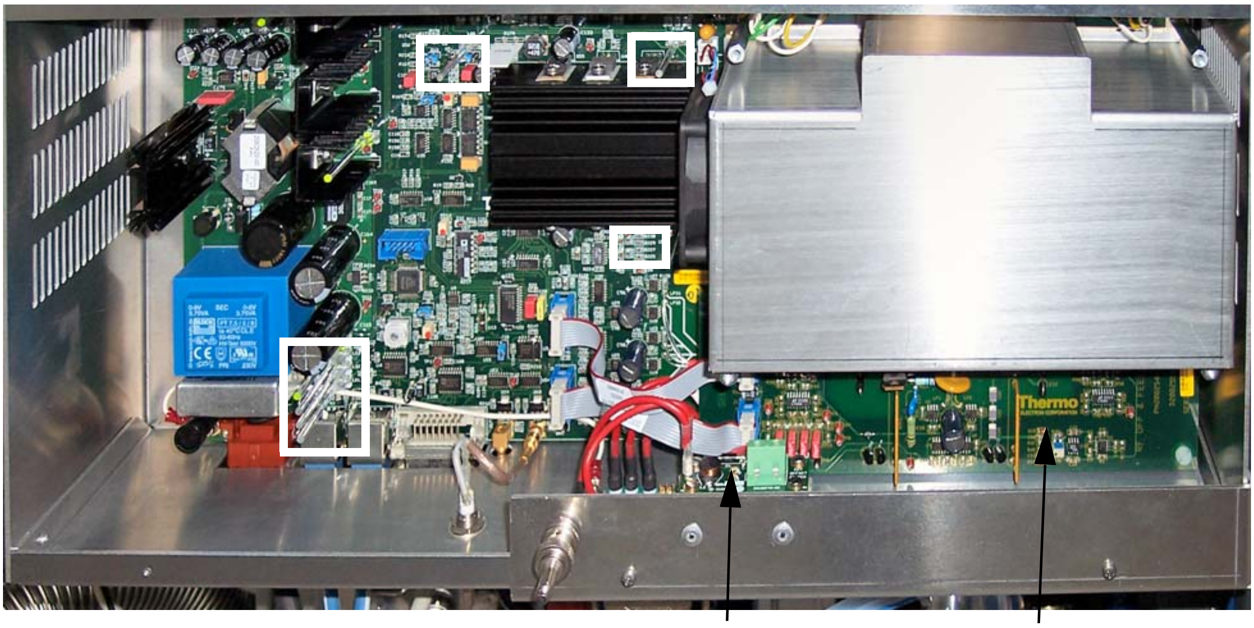


Figure 1-45. CLT RF unit (cover removed)

The diagnostic LEDs listed in Table 1-18 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 1-45.

Table 1-18. 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
LD6	OVL	Yellow	RF Amplifier overload	Off
LD7	OVHEAT	Red	Heatsink temperature > 73 °C	Off

The RF off & feedback board (P/N 208 2540) is an add-on board to the CLT RF main board. It is located in the same housing. See Figure 1-45 on page 1-63.

The CLT Offset connector (P/N 211 0470), which removes interfering signals from the circuit, is also mounted in the housing.

Central Electrode Power Supply Board

The central electrode power supply board (P/N 207 9611)[1] is mounted in a housing on the bottom left side of the instrument. See Figure 1-46.

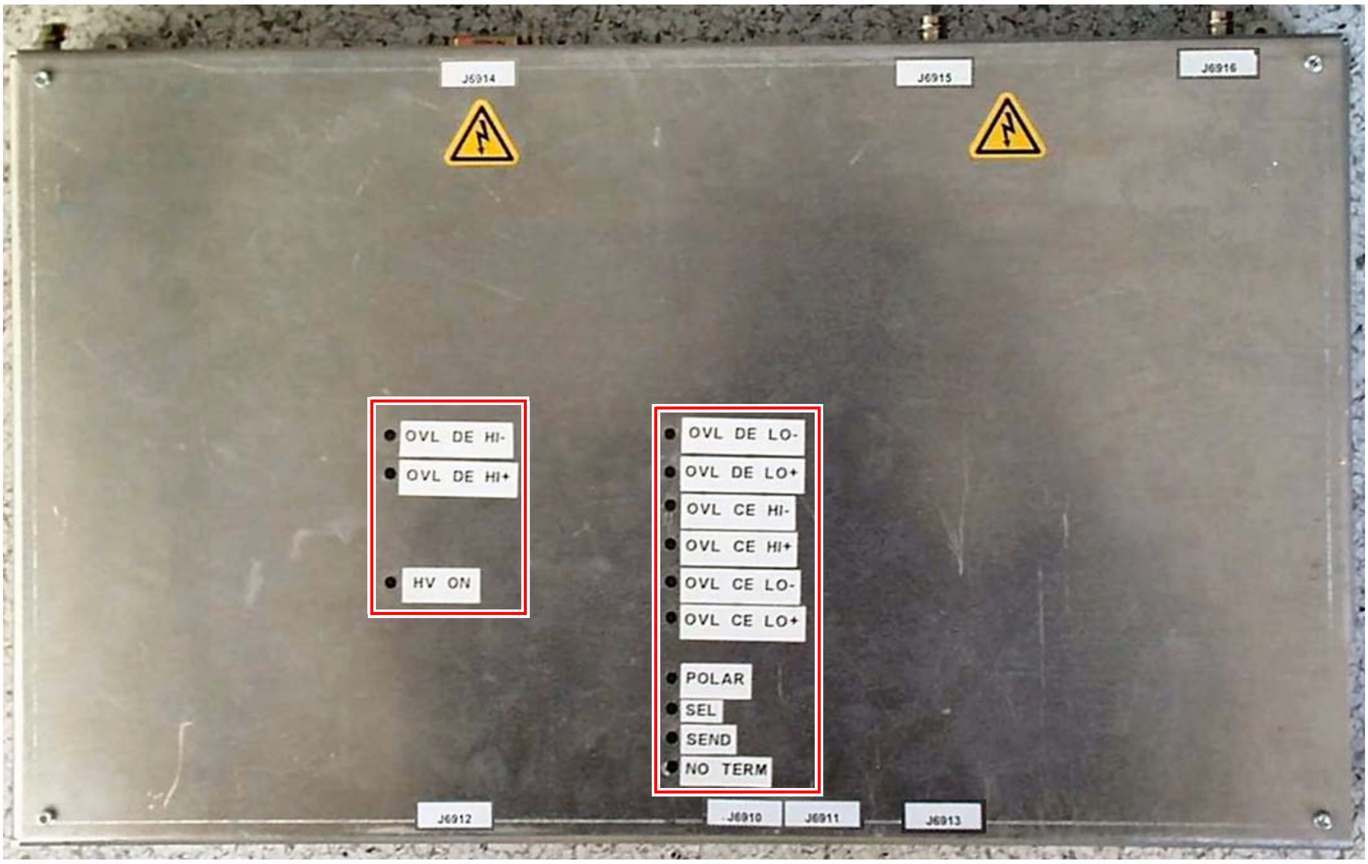


Figure 1-46. Central Electrode Power Supply board

The board supplies four dc voltages to the Orbitrap:

- 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.

[1]Part number of complete unit.

The diagnostic LEDs listed in Table 1-19 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 red rectangles in Figure 1-46.

Table 1-19. 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 (P/N 207 7991)[1] is mounted in a housing on the bottom left side of the instrument. See Figure 1-41 on page 1-58. This board provides five dc voltages for the ion optics of the LTQ Orbitrap XL ETD. Two voltages supply the lenses of the instrument. Three voltages are applied to the RF CLT main board to be

[1]Part number of complete unit.

used as focusing potentials for the curved linear trap. See topic "Orbitrap Analyzer" on page 1-13 for further information. The board communicates via the SPI bus.

Warning The high voltage power supply board creates voltages up to 3.5 kV! ▲

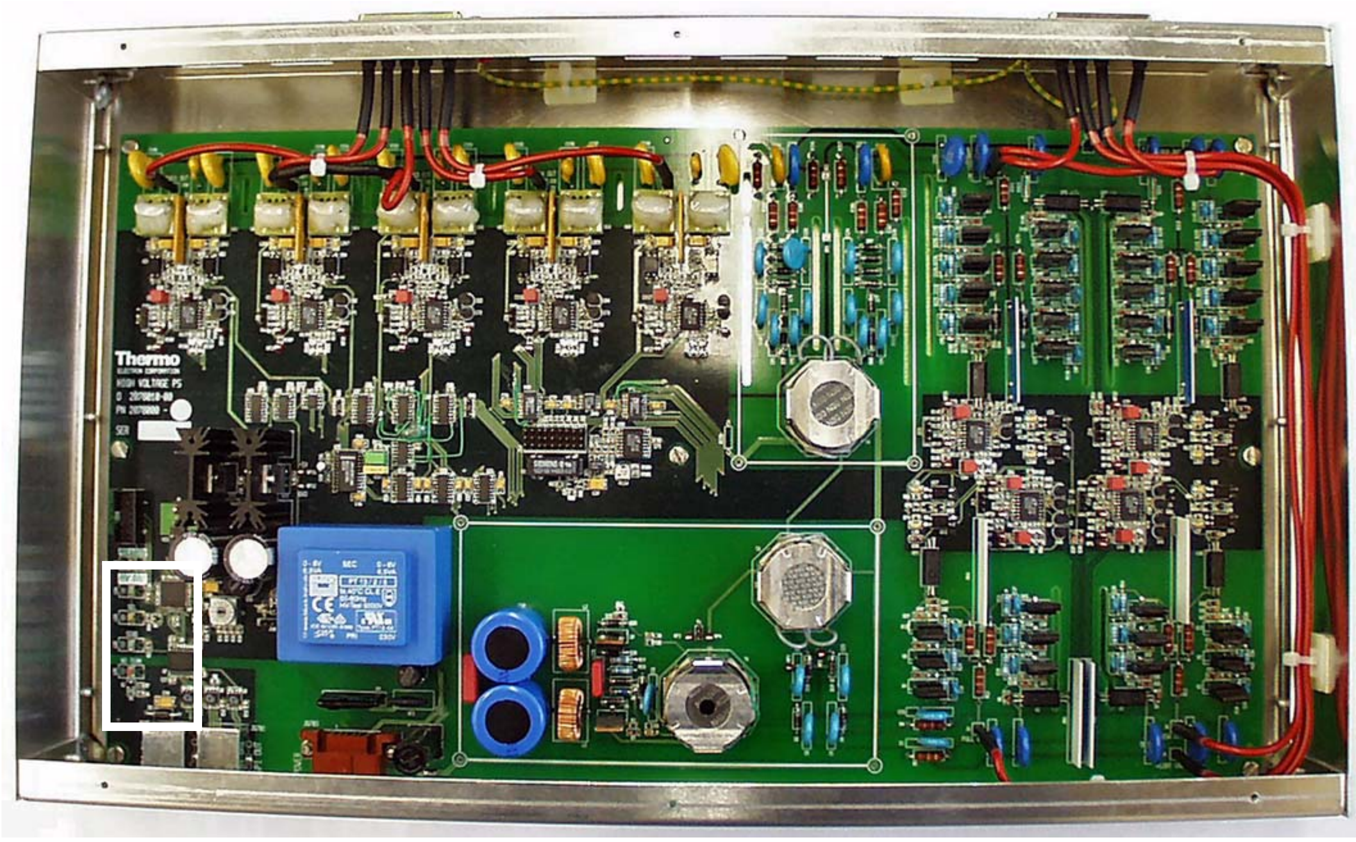


Figure 1-47. High Voltage Power Supply board (cover removed)

The diagnostic LEDs listed in Table 1-20 on page 1-67 show the operating states of the board. The position of the LEDs on the board is indicated by the white rectangles in Figure 1-47.

Table 1-20. 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 (P/N 208 1480) is located at the bottom left side of the instrument, below the High Voltage Power Supply board. See Figure 1-48.

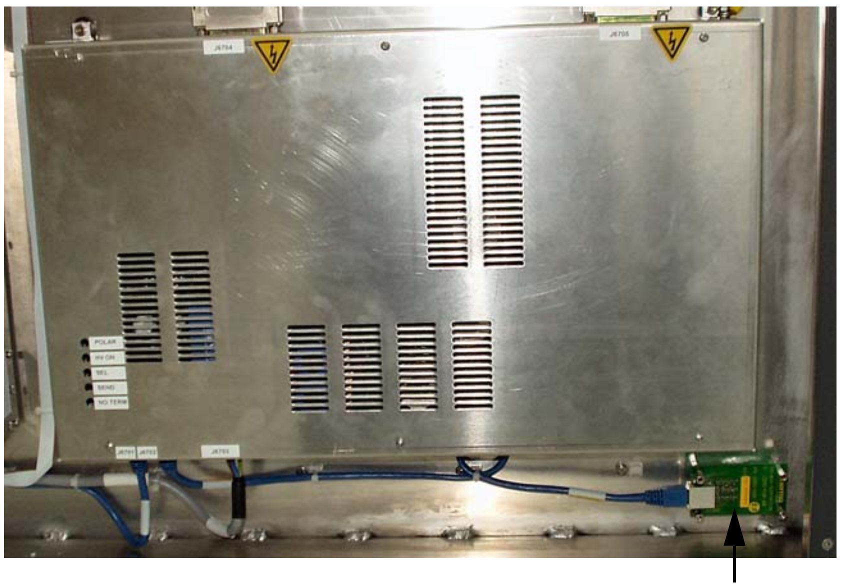


Figure 1-48. High Voltage Power Supply board with SPI Bus Termination board

Chapter 2 Basic System Operations

Many maintenance procedures for the LTQ Orbitrap XL ETD system require that the MS detector be shut down. In addition, the LTQ Orbitrap XL ETD system can be placed in Standby condition if the system is not to be used for 12 h or more.

The following topics are discussed in this chapter:

Shutting Down the System in an Emergency

If you need to turn off the MS detector in an emergency, place the main power switch (located on the power panel at the right side of the LTQ Orbitrap XL ETD) in the Off (0) position. This turns 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° anti-clockwise to switch off the instrument. See Figure 2-1.

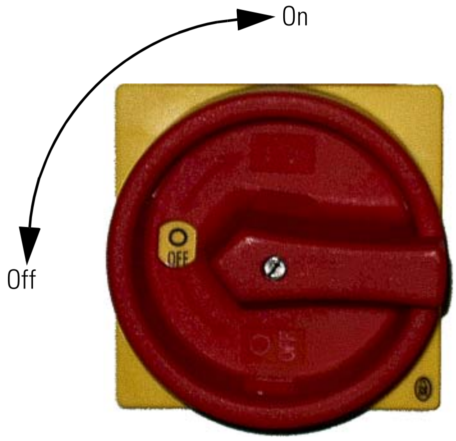


Figure 2-1. Main power switch in Off position

The instrument is automatically vented by the vent valve of the linear ion trap. The vent valve vents the system 30 s 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. Refer to topic "Shutting Down the Instrument" on page 2-7 for the recommended procedure.

Note To separately turn off the recirculating chiller or 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 via 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. Refer to the topic "Baking Out the System" on page 3-4.

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 (e.g. in the night), we recommend installing a power fail detector.

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

Placing the LTQ Orbitrap XL ETD in Standby Condition

The LTQ Orbitrap XL ETD 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.

First place the ETD Module in Standby condition and then place the mass spectrometer in Standby condition according to the procedures that follow.

Placing the ETD Module in Standby Condition

To place the ETD Module in Standby condition, do the following:

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.

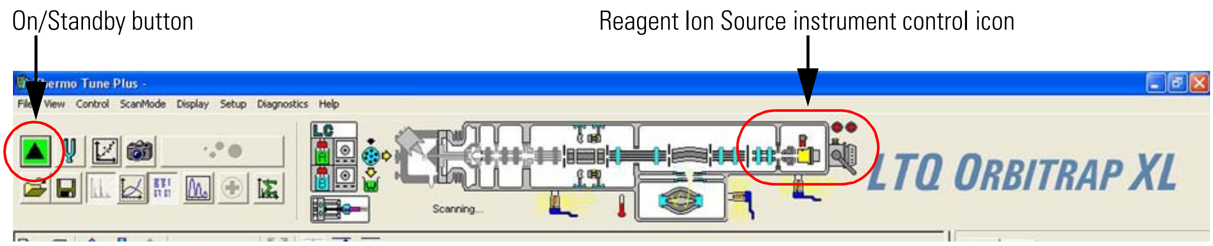
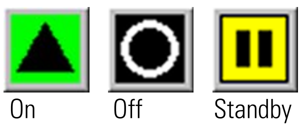


Figure 2-2. Tune Plus window, toolbar



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 2-2. 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 2-2.) The Reagent Ion Source dialog box appears. (See Figure 2-3.)

3. In the Reagent Ion Source dialog box, deselect the Reagent Ion Source On box to place the Reagent Ion Source in Standby condition. See Figure 2-3 on page 2-5. 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.

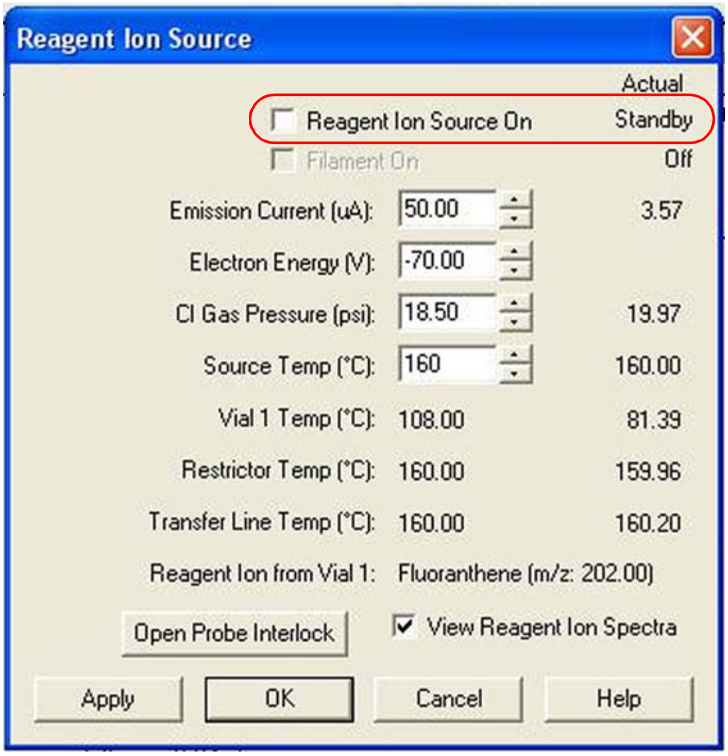


Figure 2-3. Reagent Ion Source dialog box with Reagent Ion Source On box and Actual condition circled

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.

Warning Install or exchange the reagent vials by following the procedure in topic "Changing the Reagent Vials" on page 3-48. The reagent vials will be too hot to touch after the cooling nitrogen turns off at 70°C. Verify 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 topic "Reagent Heaters" on page 1-24.

Warning The restrictor, the transfer line, and the ion source heater operate at 160 °C. Do not attempt to touch them unless the LTQ Orbitrap XL ETD is shut down (See topic "Shutting Down the LTQ Orbitrap XL ETD Completely" on page 2-7.) and these heaters have had sufficient time to cool down to room temperature. ▲

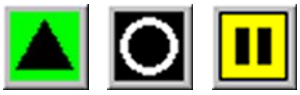
Placing the MS in Standby Condition

Use the following procedure to place the LTQ Orbitrap XL ETD 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).

Note 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 XL Hardware Manual*. The System LED on the front panel of the LTQ XL is illuminated 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 LTQ Orbitrap XL ETD main power switch in the On position.

Shutting Down the LTQ Orbitrap XL ETD Completely

The LTQ Orbitrap XL ETD 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, do the following:

1. Place the ETD Module in Standby condition as described in topic "Placing the ETD Module in Standby Condition" on page 2-4.

2. Shut down the instrument as described in topic "Shutting Down the Instrument" below. This also shuts down the ETD Module because the its power controls are linked to the LTQ Orbitrap XL ETD power controls through the ETD Module Interface board. See topic "ETD Module Interface Board" on page 1-22.

Shutting Down the Instrument

Use the following procedure to shut down the LTQ Orbitrap XL ETD 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).

Note 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 1-7 on page 1-9.

5. Put the Vacuum Pumps switch to the Off position. See Figure 1-7. 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 s, 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 LTQ Orbitrap XL ETD in the On position.

7. During service or maintenance operations that require opening the vacuum system of the LTQ XL or LTQ Orbitrap XL ETD, 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.

Warning Allow heated components to cool down before you service them (the ion transfer tube is operated at about 300 °C, for example). ▲

Note If you are planning to perform routine or preventive system maintenance on the LTQ Orbitrap XL ETD only, you do not need to turn 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 LTQ Orbitrap XL ETD 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

Note 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. ▲

Use the following procedure to start up the LTQ Orbitrap XL ETD:

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, nitrogen, and argon at the tanks, if they are off.

4. Make sure that the main power switch of the LTQ XL is in the On position and the electronics service switch of the LTQ XL is in the Operating position.

5. Place the main power switch at the right side of the LTQ Orbitrap XL ETD in the On position.

6. Put the Vacuum Pumps switch to the On position. See Figure 1-7 on page 1-9. The rotary-vane pumps and the turbomolecular pumps are started.

Note 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 1-7. 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 is illuminated yellow to indicate that the data system has started to establish a communication link.

   c. After several more seconds, the Communication LED is illuminated 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 is illuminated yellow to indicate that the software transfer from the data system is complete and that the instrument is in Standby condition.

Note The Vacuum LED on the front panel of the LTQ XL is illuminated 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 capillary-skimmer 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 LTQ XL to establish the communication link between LTQ XL 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 topic “Setting Up Conditions for Operation“ below. If you do not have either, go to the topic directly.

Setting Up Conditions for Operation

Set up your LTQ Orbitrap XL ETD for operation, as follows:

1. Before you begin data acquisition with your LTQ Orbitrap XL ETD 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.

Note The vacuum in the analyzer system can be improved by an overnight baking of the system. Refer to the topic "Baking Out the System" on page 3-4. ▲

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),
   - Argon: 690 ± 140 kPa (6.9 ± 1.4 bar, 100 ± 20 psi).

Note 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. Continue to set up for ESI or APCI operation as described in *LTQ Orbitrap XL Getting Started* manual.

Starting the ETD Module After a Complete Shutdown

To start up the ETD Module after a complete shutdown, do the following:

1. Start the LTQ Orbitrap XL ETD according to the start up procedures given in topic "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 topic "ETD Module Interface Board" on page 1-22).

2. 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.

On Off Standby

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 2-2 on page 2-4.) The three different states of the On/Standby button are shown at the left.

Resetting the System

If the communication link between LTQ Orbitrap XL ETD and data system computer is lost, it may be necessary to reset the system using the Reset button of the LTQ XL.

The procedure given here assumes that the LTQ Orbitrap XL ETD and data system computer are both powered on and are operational. If the instrument, data system computer, or both are off, refer to topic "Starting Up the System after a Shutdown" on page 2-9.

To reset the LTQ Orbitrap XL ETD, press the Reset button of the LTQ XL. See the *LTQ XL 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 is illuminated 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 is illuminated 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 min, the software transfer is complete. The System LED is illuminated 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 the Tune and Calibration Parameters to their Default Values

You can reset the LTQ Orbitrap XL ETD 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 LTQ Orbitrap XL ETD tune and calibration parameters to their default values, proceed as follows:

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.

Note 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

The reagent ion source controls can be accessed as described in topic "Placing the ETD Module in Standby Condition" on page 2-4. When you deselect the Reagent Ion Source On check box in the Reagent Ion Source dialog box (See Figure 2-4.), the ETD source and reagent heaters are placed in Standby condition.

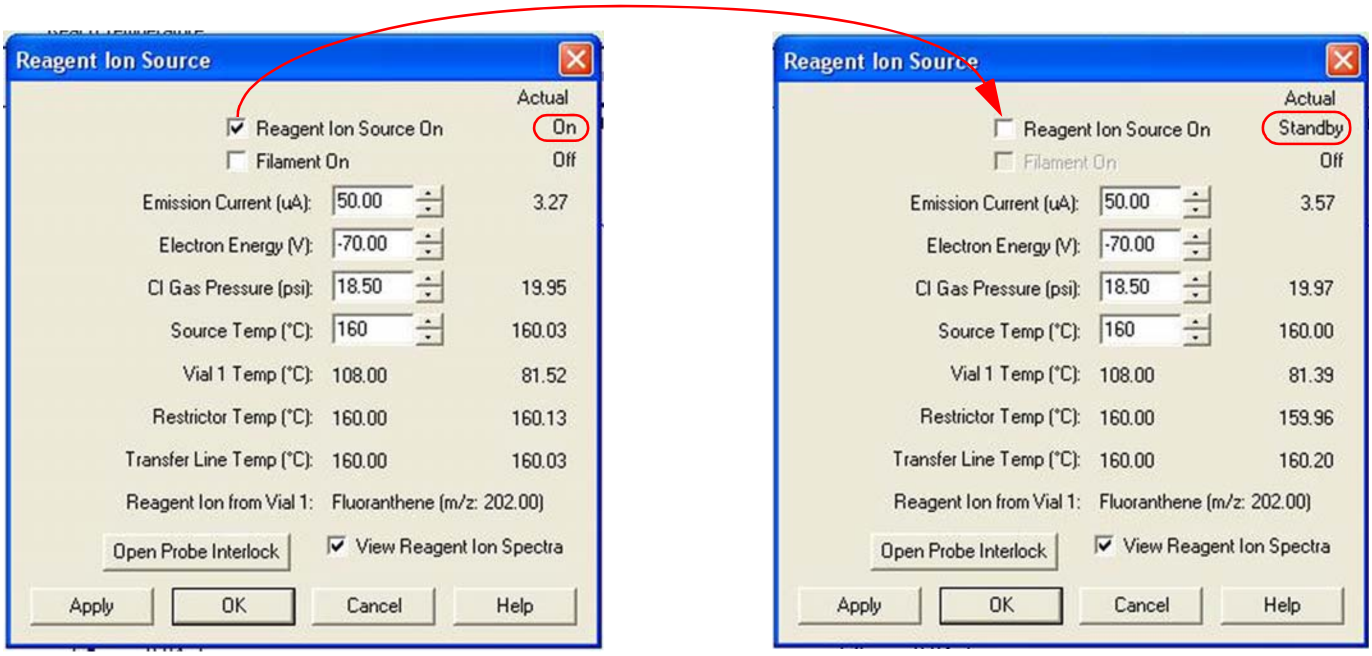


Figure 2-4. Placing the reagent ion source in Standby condition

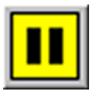
When the ETD Module is placed in Standby condition, the filament and vial heaters are turned off. Simultaneously a valve opens to allow nitrogen gas to cool the reagent vials. This cooling nitrogen runs until the vials reach 70 °C. The audible rush (hissing noise) of nitrogen from the reagent ion source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

Warning The reagent vials are too hot to handle after the cooling nitrogen turns off at a vial temperature of 70 °C. Verify 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:

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

- Whenever 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 LTQ Orbitrap XL ETD 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. ▲

- Whenever 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.

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

Chapter 3 User Maintenance

This chapter describes routine maintenance procedures that must be performed to ensure optimum performance of the LTQ Orbitrap XL ETD.

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

The following topics are described in this chapter:

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

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 3-1.

Table 3-1. User maintenance procedures

MS Detector Component	Procedure	Frequency	Procedure Location
Analyzer	System bakeout	If necessary (e.g. after performing maintenance work on the vacuum system)	page 3-4
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
Turbomolecular pumps	Exchange lubricant reservoir	Once a year	Manufacturer's documentation page 3-12
Recirculating chiller	Check cooling fluid level Check cooling fluid filter Check air inlet filter	See manufacturer's documentation	Manufacturer's documentation page 3-61
ETD Module	Clean the ion volume	As needed*	page 3-19
	Replace the inlet valve components	As needed*	page 3-46
	Clean the ion source lenses	As needed*	page 3-34
	Clean the ion source	As needed*	page 3-41
	Replace the ion source filament	As needed*	page 3-43
	Check the rotary-vane pump oil and add when needed	Every month	page 3-8
	Change the rotary-vane pump oil	Every 4 months	page 3-10
	Clean the rear cooling fans	Every four months	page 3-60

* 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.

- 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 whenever you remove the top cover plate of the vacuum manifold.
- Never overtighten a screw or use excessive force.
- Dirty tools can contaminate your system. Keep the tools clean and use them exclusively for maintenance and service work at the LTQ Orbitrap XL ETD.
- Never insert a test probe (for example, an oscilloscope probe) into the sockets of female cable connectors on PCBs.

Returning Parts

In order to protect our employees, we ask you for some special precautions when returning parts for exchange or repair to the factory. Your signature on the Repair Covering letter confirms that the returned parts have been de-contaminated and are free of hazardous materials. Refer to topic "Safety Advice for Possible Contamination" on page ix for further information.

Cleaning the Surface of the Instrument

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

Caution Prevent any liquids from entering the inside of the instrument. ▲

Maintenance of the Vacuum System

This sections 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 noticeable during routine operation.

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

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

In case the system has been vented during a power failure, it is necessary to bake out the system to obtain the operating vacuum. Refer to the topic "Behavior of the System in Case of a Main Failure" on page 2-2.

Bakeout Procedure

Use the following procedure to perform a system bakeout:

1. Place the system in Standby condition as described in topic "Placing the LTQ Orbitrap XL ETD in Standby Condition" on page 2-4.

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

Figure 3-1. Bakeout timer

3. Set the bakeout time by entering the desired time (hh:mm) with the up/down keys of the bakeout timer. See Figure 3-1 on page 3-4.

4. Start the bakeout procedure by pressing the green start button on the right. The LTQ Orbitrap XL ETD indicates a running bakeout procedure by the flashing Vacuum and System LEDs on the front side of the instrument. See Figure 1-4 on page 1-6.

You can stop a running bakeout procedure by pressing 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.

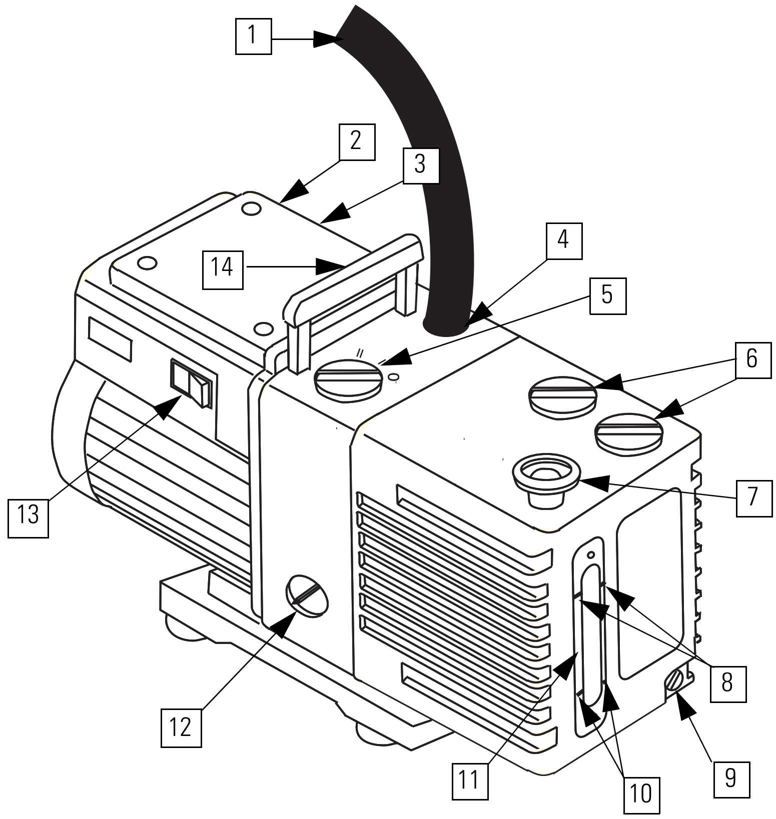
For maintenance of the forepumps of the MS portion, refer to the *LTQ XL Hardware Manual* or the pump manufacturer's manual.

Note 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 (P/N A0301-15101) 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 3-2.



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 3-2. Schematic of ETD forepump

Note 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 topic "Forevacuum Pump of the ETD Module" on page 1-32, 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 3-3.

Figure 3-3. 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 3-4 shows the details for the right side of the instrument.

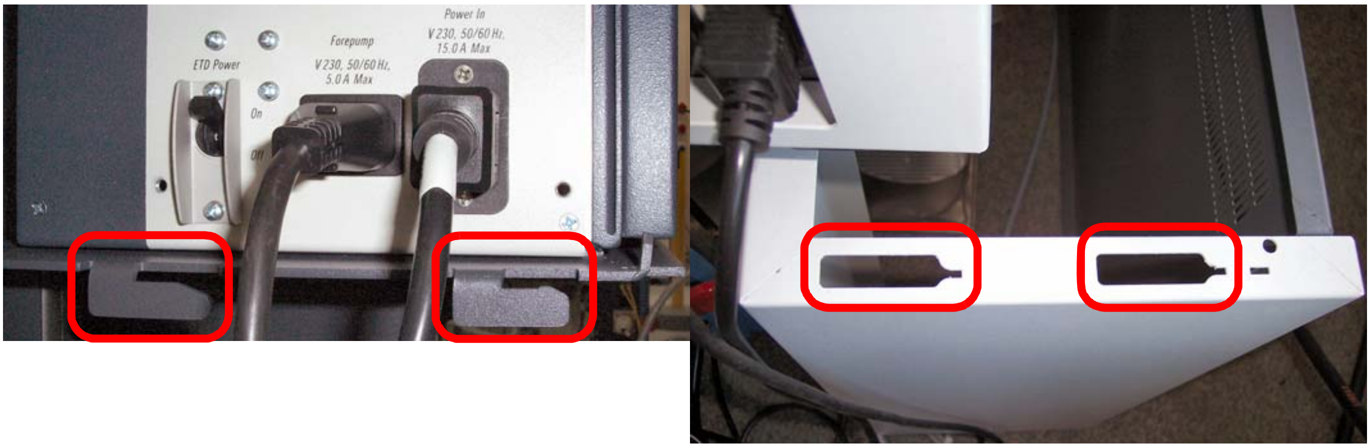


Figure 3-4. Hooks (left) and top side of detached bottom panel (right)

On the bottom of the rear side of the MS portion, two Allen screws fix the panel to the instrument frame by means of fork-like extensions (lugs). See Figure 3-5.

Figure 3-5. Lugs for fixing the bottom panel

To remove the panel, do the following:

1. Use a 6 mm Allen 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 (P/N A0301-15101) 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 3-2. If the ETD forepump oil level is low, follow these steps to add more oil.

To add oil to the ETD forepump, do the following:

1. Shut down and vent the LTQ Orbitrap XL ETD.

Caution 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 3-8.

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

Caution 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.

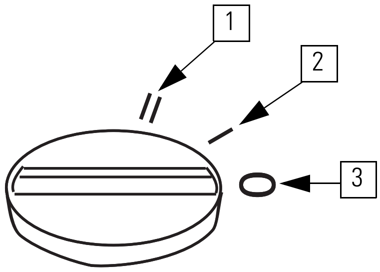
To purge the rotary-vane pump oil, do the following:

1. Remove the lower panel at the rear side of the ETD Module as described on page 3-8.

2. Set the gas ballast control (See Figure 3-2.) 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 (O), as shown in Figure 3-6.



Labeled components: 1=High Flow (Position II), 2=Low Flow (Position I), 3=Closed (Position O)

Figure 3-6. 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 (P/N A0301-15101)
- Suitable container for removing spent or excess oil

Note For best results, change the oil while the ETD forepump is still warm after operation. Be careful, however, as the oil can still be very hot at this time. ▲

Warning **Danger of Burns.** Handle hot pump oil carefully to avoid being burned or injured. ▲

To change the ETD forepump oil, do the following:

1. Shut down and vent the LTQ Orbitrap XL ETD.

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

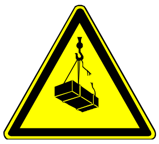
2. Remove the lower panel at the rear side of the ETD Module as described on page 3-8.

3. Disassemble the rotary-vane pump.

   a. Disconnect the foreline vacuum hose. (See Figure 3-2.)

   b. Disconnect the exhaust vacuum hose.

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



Warning **Lifting Hazard.** Use the proper lifting technique to lift the ETD forepump. It weighs approximately 50 pounds (22.7 kg). ▲

4. Drain the spent oil.

   a. Remove one of the oil filler plugs.

   b. Remove the oil drain plug and allow the oil to 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 Turbopumps

The turbopumps in the MS portion of the LTQ Orbitrap XL ETD need maintenance work that is briefly outlined below. In contrast, the turbopump in the ETD Module contains no user-serviceable parts.

Note 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! ▲

Exchanging the Lubricant Reservoir of the Turbopumps

Note For all manipulations at the pumps, note the advice, warnings, and cautions contained in the pump manuals! ▲

For the turbopumps, we recommend exchanging the lubricant reservoir once per year. At each exchange procedure, the complete lubricant reservoir must be exchanged!

Note The storage stability of the lubrication oil is limited. The specification of durability is given by the pump manufacturer. (Refer to the manuals for the turbopumps.) ▲

Replacements for the turbopump lubricant reservoirs (TMH 071 P: P/N 017 2350; TMU 262: P/N 105 0160) are available from Thermo Fisher Scientific.

The disposal of used oil is subject to the relevant regulations.

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.

Figure 3-7 illustrates the sequence in which to perform routine maintenance on the ETD System.

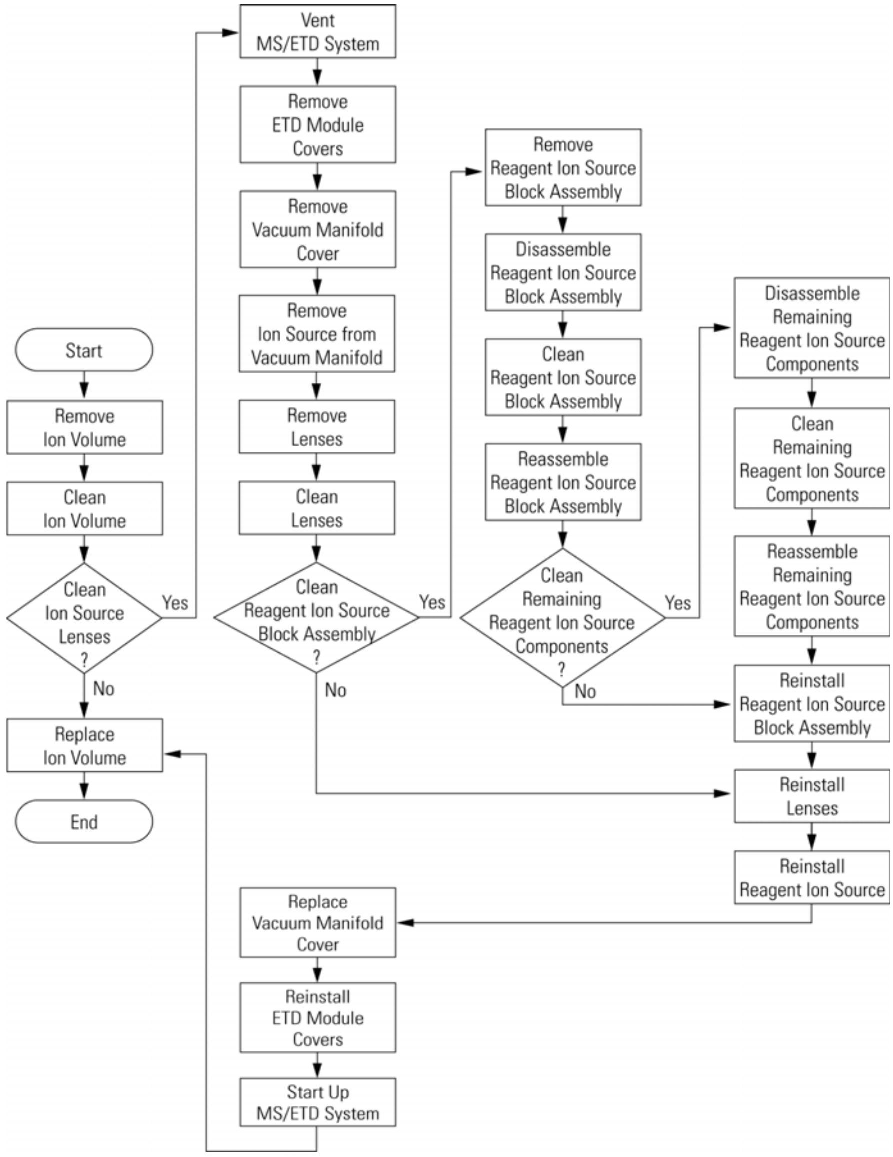


Figure 3-7. Routine maintenance sequence for ETD system

Requirements for 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 doing 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 3-1 on page 3-2). 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 you have all the necessary tools before carrying out a procedure. See below for a list of the tools and supplies 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.

Note 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, 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)
- Gloves, clean, lint- and powder-free
- Gloves, nitrile
- Lint-free cloth or paper
- Nut driver, 5.5 mm
- Protective eyewear
- Screwdriver, Phillips #2
- Screwdriver, flat blade
- Wrench, adjustable

- Wrench, Allen, 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. These parts are cleaned by following the procedure described in this topic. Use this procedure with caution because some components can be damaged when exposed to liquids.

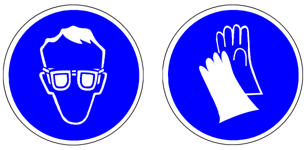
The following tools and supplies are needed for cleaning stainless steel parts in the reagent ion source:

- Acetone, analytical grade (or other suitable solvent)
- Aluminum oxide abrasive, number 600 (P/N 32000-60340)
- Applicators, cotton-tipped (P/N A0301-02000)
- Beaker, 450 mL
- Clean, dry gas
- De-ionized water
- Detergent (Alconox, Micro, or equivalent)
- Dremel rotary tool or equivalent (recommended)
- Foil, aluminum
- Forceps
- Gloves, clean, lint- and powder-free
- Gloves, nitrile
- Glycerol, reagent grade
- Lint-free cloth
- Protective eyewear
- Tap water

- Toothbrush, soft
- Ultrasonic cleaner

Caution Do not use this procedure to clean ceramic, aluminum, or gold plated parts. See page 3-17 for the method for cleaning ceramic, aluminum, or gold plated parts. ▲

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



Warning Wear impermeable laboratory gloves and eye protection when performing these cleaning procedures. ▲

To clean reagent ion source stainless steel parts, do the following:

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 appears as dark or discolored areas, but may 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.

Warning To prevent personal injury, be sure to keep the Dremel tool away from possible hazards, such as standing water or flammable solvents. ▲

2. Rinse the parts with clean water. 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.

3. Place the parts in a warm detergent solution in an ultrasonic bath and sonicate them.

    a. Using forceps, place the parts in a beaker containing warm detergent solution.

    b. Place the beaker and contents in an ultrasonic bath for five minutes.

    c. Rinse the parts with tap water to remove the detergent.

4. Sonicate the parts in deionized water.

    a. Using forceps, 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.

5. Sonicate the parts in acetone.

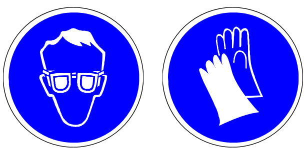
    a. Using forceps, place the parts in a beaker containing fresh acetone.

    b. Place the beaker and contents in an ultrasonic bath again for five minutes.

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

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 3-16. Perform these steps only on the stainless-steel surfaces of hybrid parts. Do not allow the aluminum oxide slurry to contact the aluminum, ceramic, or gold plated portions of these parts.



Warning Wear impermeable laboratory gloves and eye protection when performing the following cleaning procedures. ▲

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, do the following:

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

   a. Scrub the parts with a toothbrush or clean applicator. Do not soak or sonicate the parts in detergent.

   b. Using forceps, rinse the parts thoroughly with tap water to remove the detergent.

Caution 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. Using forceps, 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. Using forceps, 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.

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 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.

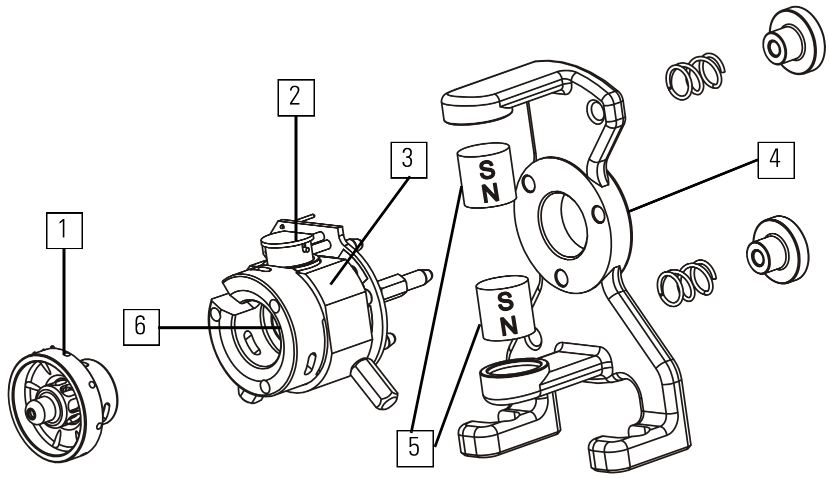
To restore system performance, always clean the ion volume first, then the ion source lenses. If cleaning either of these components does not restore system performance, try cleaning the entire reagent ion source.

This section contains these maintenance procedures:

- "Cleaning the Ion Volume With an Inlet Valve" on page 3-19
- "Cleaning the Ion Source Lens Assembly" on page 3-34

- "Cleaning the Ion Source" on page 3-41
- "Replacing the Ion Source Filament" on page 3-43
- "Replacing Inlet Valve Components" on page 3-46

The ion source, the ion trap, and their components are shown in Figure 3-8.



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 3-8. Ion source components (left view)

Cleaning the Ion Volume With an Inlet Valve

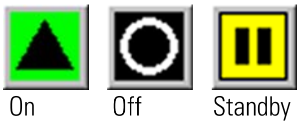
The ion volume is where molecules interact with energetic electrons to form ions. Because the ion volume is exposed directly to reagents introduced into the reagent ion source, you will have to clean it more frequently than other parts. How often you have to clean the ion volume assembly will depend 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 topic "Cleaning Stainless Steel Parts" on page 3-15.)
- Gloves (clean, lint-free, and powder-free)
- Ion volume tool and guide bar
- Lint-free cloth

Using the ion volume tool allows you 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, do the following:



1. Click the On/Standby button in the Tune Plus window to place the LTQ Orbitrap XL ETD in Standby mode. See Figure 3-9.

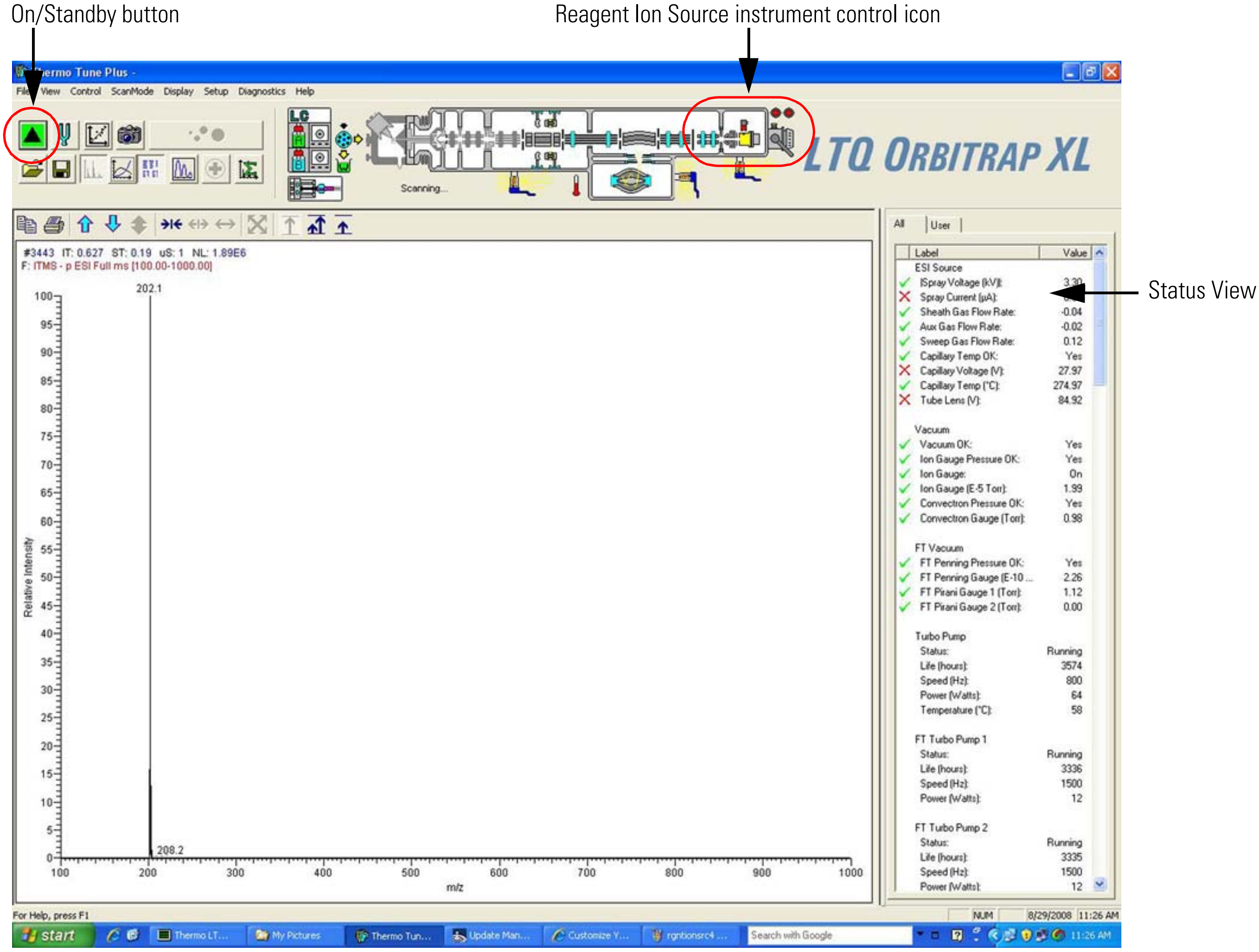
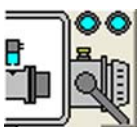
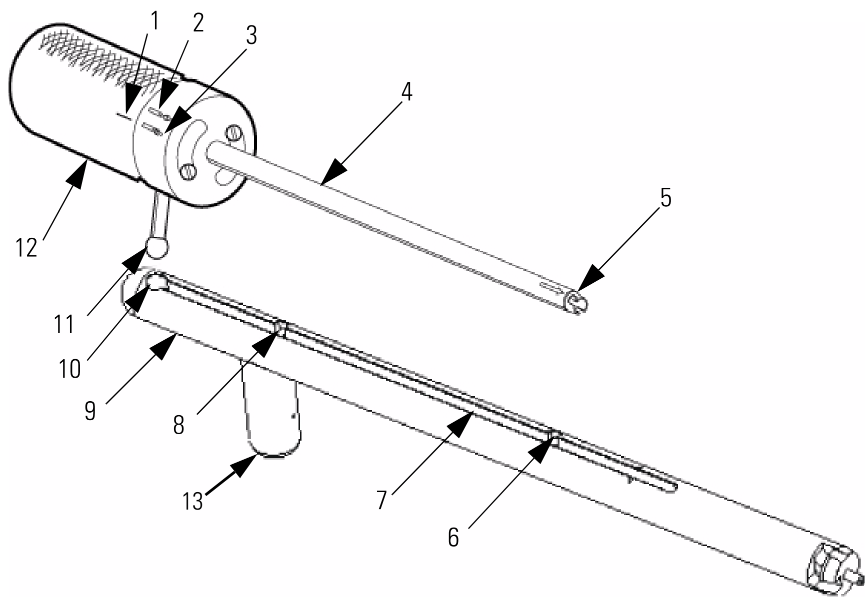


Figure 3-9. Tune Plus window



2. Open the Reagent Ion Source dialog box (Figure 3-16 on page 3-25) in Tune Plus by clicking the Reagent Ion Source instrument control icon.



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 3-10. Ion volume tool components

3. Place the guide bar handle (item 13 in Figure 3-10 on page 3-21) to the 3 o'clock position (Figure 3-11 on page 3-21).

4. Insert the guide bar (item 9 in Figure 3-10) into the guide bar opening in the back of the ETD Module (Figure 3-11).

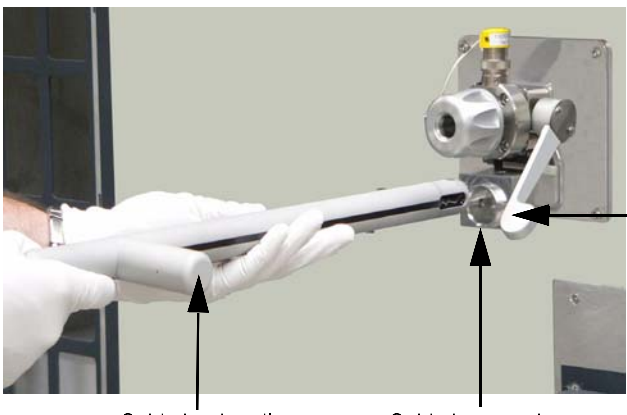


Figure 3-11. Guide bar being inserted into guide bar opening*

*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 3-12). The guide bar handle faces the floor at the completion of this step.

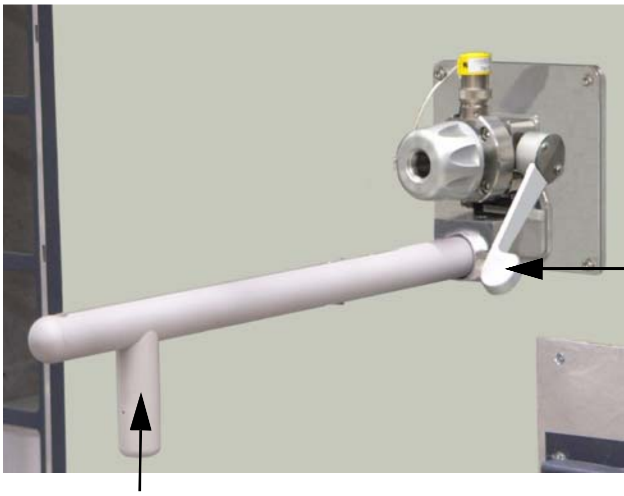
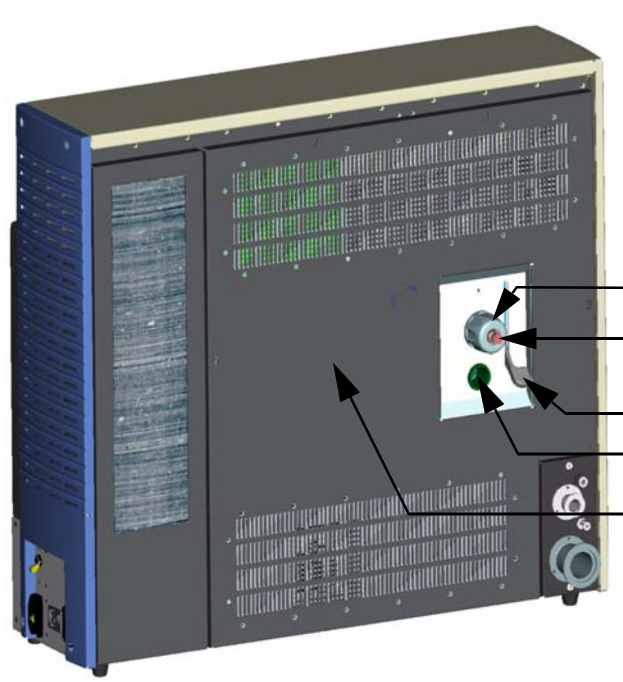


Figure 3-12. Guide bar insertion complete*

*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.

   Make sure the inlet valve is closed (inlet valve lever is down, as shown in Figure 3-12) and remove the inlet valve plug (item 2 in Figure 3-13). Do this by rotating (loosening) the inlet valve knob (item 1 in Figure 3-13 on page 3-23) until the inlet valve plug (item 2 in Figure 3-13) will slide out easily. The inlet valve plug prevents air from entering the vacuum manifold in case the inlet valve is inadvertently opened.



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 3-13. Rear view of the ETD Module, showing the inlet valve

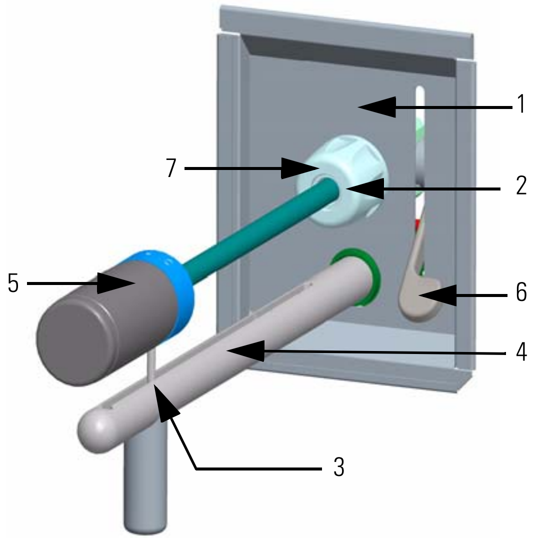
7. Turn the ion volume tool handle to the unlock position, which indicates that the ion volume tool is in position to accept the ion volume. See Figure 3-14.

Figure 3-14. 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.

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 3-10 on page 3-21 and Figure 3-15.



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 3-15. Ion volume tool guide bar first stop

c. Slide the ion volume tool so the guide ball is in the groove at the first stop (Figure 3-10 on page 3-21 and Figure 3-15). This prevents the probe from being pulled forward when the inlet valve is evacuated.

d. Tighten the inlet valve knob (Figure 3-15) to ensure that a leak-tight seal is made.

e. Click **Open Probe Interlock** in the Reagent Ion Source dialog box (Figure 3-16). A message box appears 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, replace the inlet valve seal as described in topic "Replacing Inlet Valve Components" on page 3-46. When the target pressure is achieved, a message appears stating that the ball valve can be opened (Figure 3-17).

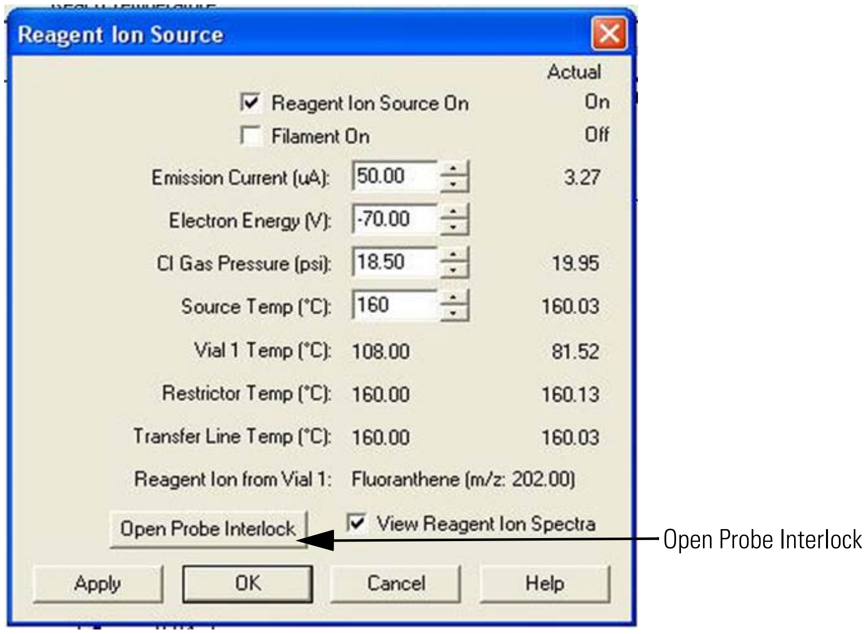


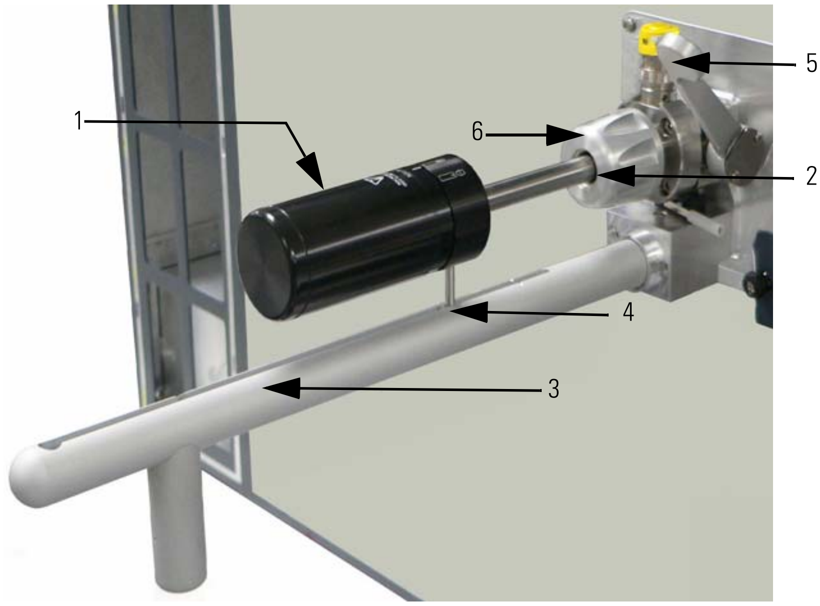
Figure 3-16. Reagent Ion Source dialog box, Open Probe Interlock button.

Figure 3-17. Instrument Message box: The Ball Valve can now be opened

f. Once evacuation is complete, push up the inlet valve lever to open the inlet valve (Figure 3-18).

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 3-18.



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 3-18. Ion volume tool 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 3-10 on page 3-21) will be just past the first mark on the guide bar as shown in Figure 3-19.

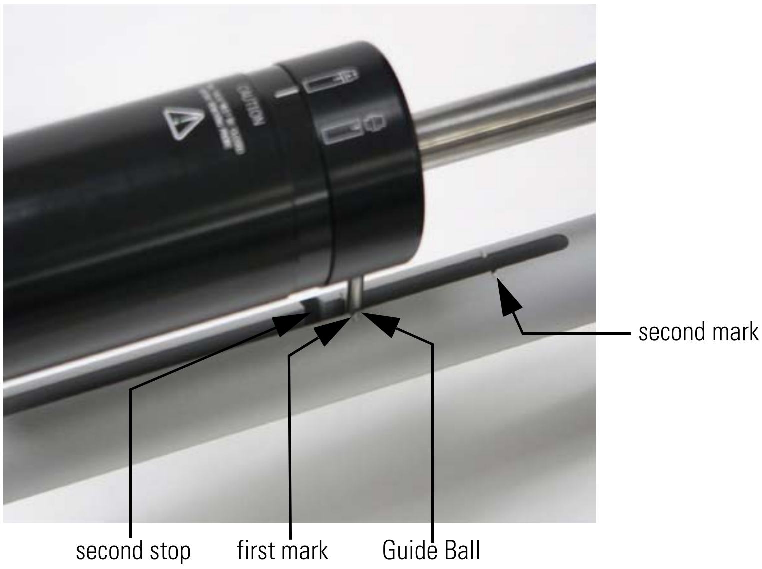


Figure 3-19. Detail of ion volume tool fully inserted into the inlet valve

b. Turn the ion volume tool handle counterclockwise to the lock position, See Figure 3-20. Listen for a click indicating that the handle is fully engaged in the lock position and is holding the ion volume.

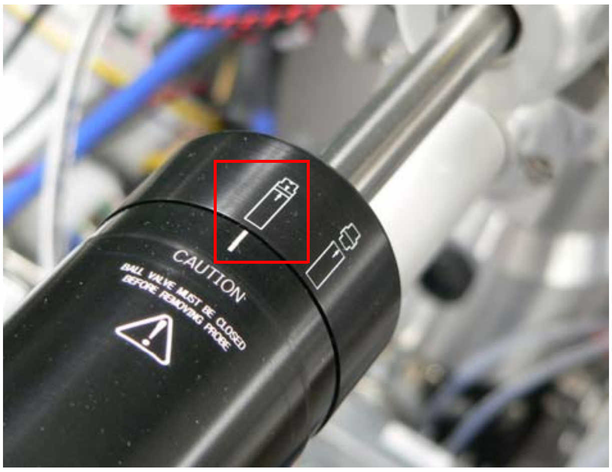


Figure 3-20. Ion volume tool handle in the locked position

c. Withdraw the ion volume tool (the ion volume is attached) until the guide ball reaches the first stop (see Figure 3-10 on page 3-21 and Figure 3-15 on page 3-24 for the first stop position).

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

Caution 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 withdrawing the ion volume tool past the first stop. Otherwise, the system will vent to the atmosphere and cleaning the components under vacuum will be required. ▲

e. Loosen the inlet valve knob (Figure 3-18).

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.

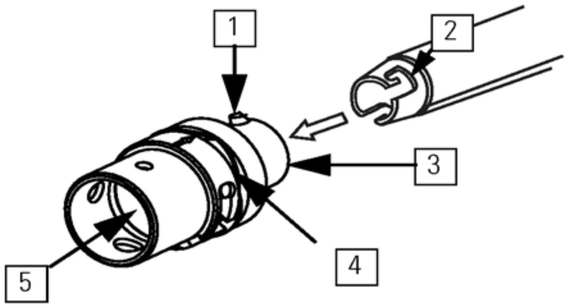
Warning The ion volume will be too hot to touch. Let it cool to room temperature before handling it. ▲

10. Clean the ion volume:

a. Turn the ion volume tool handle to the unlock position (Figure 3-14 on page 3-23). 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 3-21.



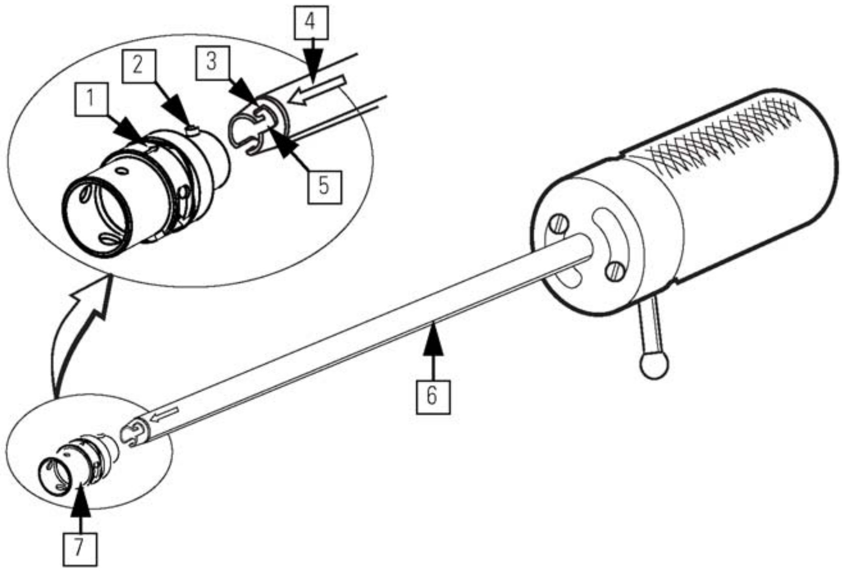
Labeled components: 1=bayonet pin, 2=bayonet pin guide, 3=ion volume holder, 4=spring washer, 5=ion volume

Figure 3-21. Ion volume assembly

c. Clean the ion volume and ion volume holder according to the instructions in topic "Cleaning Stainless Steel Parts" on page 3-15.

11. 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 3-22.



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 3-22. Placing the ion volume on the ion volume tool

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

b. Slide the ion volume tool handle to the lock position. (See Figure 3-20 on page 3-27.)

Caution The arrows on the ion volume tool and ion volume must be aligned to avoid damage to the ion source.

12. 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 3-10 on page 3-21 and Figure 3-15 on page 3-24).

b. Turn the ion volume tool so that the guide ball is in the groove at the first stop (Figure 3-15 on page 3-24). 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 3-18 on page 3-26).

d. Click **Open Probe Interlock** in the Reagent Ion Source dialog box (Figure 3-16 on page 3-25). 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 topic "Replacing Inlet Valve Components" on page 3-46. When the target pressure is achieved, a message will appear stating that the ball valve can be opened. See Figure 3-17 on page 3-25.

e. Once evacuation is complete, push the inlet valve lever up to open the inlet valve. See Figure 3-18 on page 3-26.

13. Reinsert the ion volume:

a. Slide the ion volume tool into the vacuum manifold, as illustrated in Figure 3-18.

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 3-19 on page 3-26.

c. Turn the ion volume tool handle to the unlock position. See Figure 3-23.

Figure 3-23. 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 3-24 on page 3-30.

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 3-10 on page 3-21 and Figure 3-15 on page 3-24).

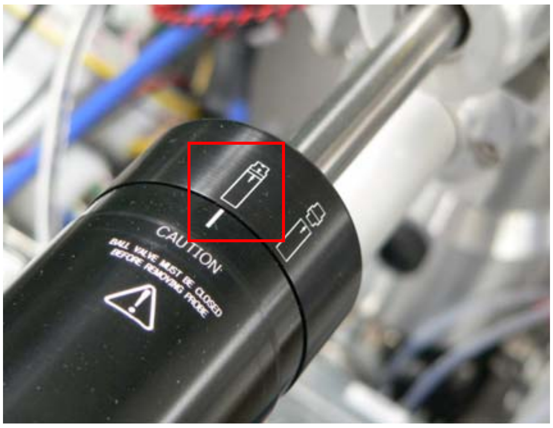


Figure 3-24. Ion volume tool handle in the locked position

e. Close the inlet valve by pushing down on the inlet valve lever (Figure 3-13 on page 3-23).

Caution 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 withdrawing 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 3-18 on page 3-26).

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.

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

    a. Remove the guide bar by rotating it 90º counter-clockwise and sliding it out of the entry housing.

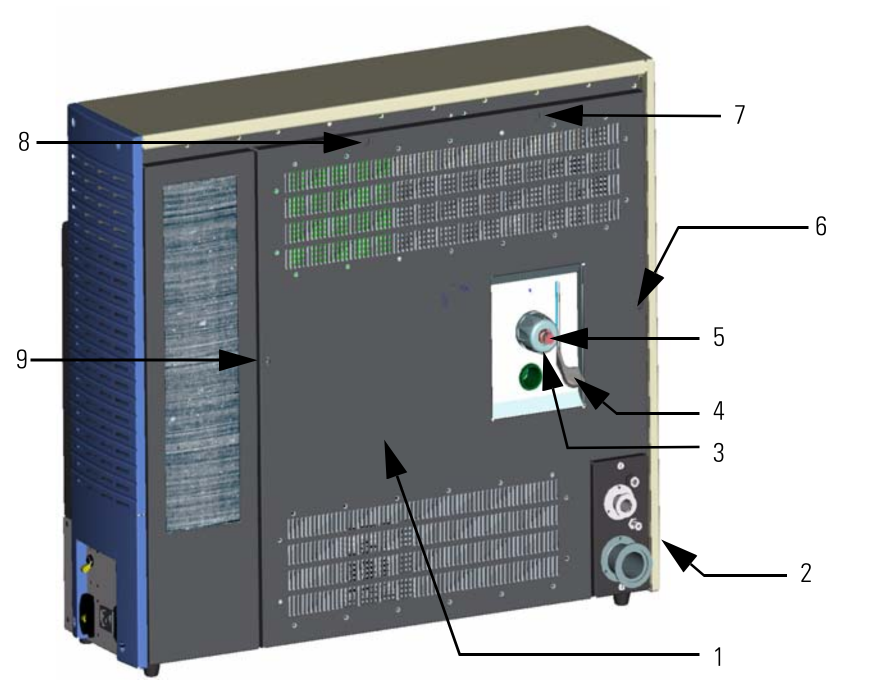
    b. Replace the inlet valve plug and tighten the inlet valve knob (item 6 in Figure 3-18 on page 3-26).

    c. Click **Close** in the message stating that the ball valve can be opened. (See Figure 3-17 on page 3-25.)

Note 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. ▲

Removing the ETD Main Access Panel

During some ETD Module maintenance activities it is necessary to remove either the ETD main access panel or side access panel or both (see Figure 3-25). 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 3-25. Rear view of the ETD Module

To remove the ETD main access panel, do the following:

1. Place the ETD Module to Service mode as directed in topic "Place the Instrument in Off Condition and Service Mode" on page 3-49.

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

Warning 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 may be too hot to touch. Verify that all of these components are safe to touch before handling them. ▲

Note 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 3-25 on page 3-32) 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.

Caution Rotating the inlet valve lever upwards (to the open position) without the inlet valve plug (item 5 in Figure 3-25) or the ion volume tool in place will cause a catastrophic venting of the system. ▲

3. Remove the inlet valve knob (item 3 in Figure 3-25) and the inlet valve plug (item 5 in Figure 3-25) by unscrewing the inlet valve knob. Be sure that the inlet valve lever (item 4 in Figure 3-25) remains in the down position.

4. Remove the four panel fasteners (items 6, 7, 8, and 9 in Figure 3-25).

5. Tilt the top of 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, do the following:

1. If it is not already in Service mode, place the ETD Module in Service mode as directed in topic "Place the Instrument in Off Condition and Service Mode" on page 3-49.

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

Warning 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 may be too hot to touch. Verify that all of these components are safe to touch before handling them. ▲

Note 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 turbo pump will continue operating. ▲

2. Remove the grey plastic panel by removing the four screws that hold it in place.

3. Remove the metal side access panel (item 2 in Figure 3-42 on page 3-52) by removing the three screws that hold it in place.

Warning Reagent vial heaters, ion source heater, flow restrictor, and transfer lines are accessible under the ETD side access panel. These are heated components. Verify 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.

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 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, do the following:

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 2-7).

Caution Shut down and unplug the LTQ Orbitrap XL ETD before proceeding with the next steps of this procedure. ▲

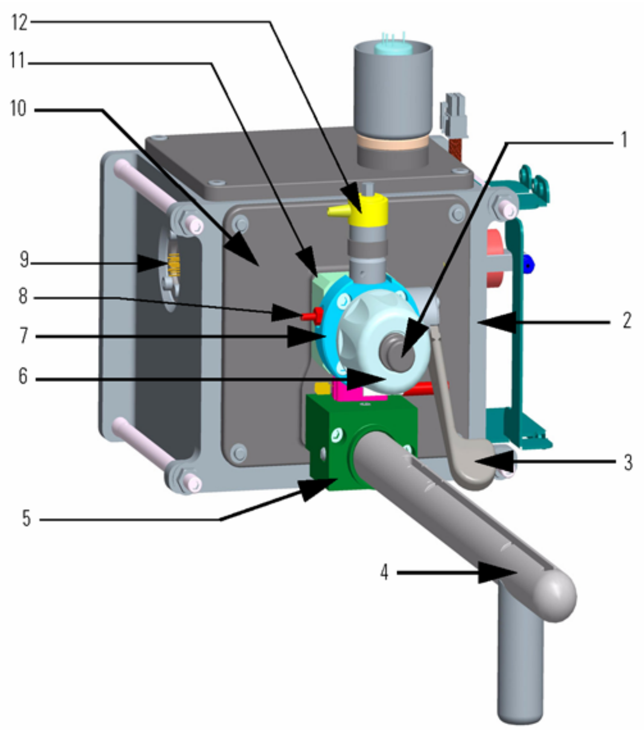
Note Wear clean, lint- and powder- free gloves when you handle parts inside the vacuum manifold. ▲

Warning The ion source may be too hot to touch even if the cooling nitrogen has completed its cycle. Be sure that the ion source has cooled to room temperature before handling it. ▲

2. Remove the ion source assembly:

a. Remove the main access panel of the ETD Module (item 1 in Figure 3-25 on page 3-32). Follow the procedures in topic "Removing the ETD Main Access Panel" on page 3-31.

Caution It is good practice to keep the inlet valve lever in the down (closed) position whenever 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 accidently lost the system may 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 3-26. Inlet valve components (ion volume tool not shown)

b. Remove all connectors between the components on the vacuum manifold probe plate (item #10, Figure 3-26 on page 3-35) and the ETD Control PCB (Figure 1-15 on page 1-20).

c. Remove the valve shield from the vacuum manifold probe plate (Figure 3-27) by loosening the four screws at the corners of the shield.

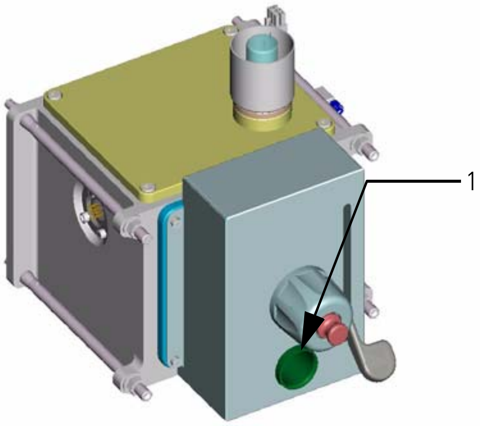


Figure 3-27. Valve shield (1) covering the vacuum manifold probe plate

d. Remove the foreline hose on the source from its connection (Figure 3-28 and item 8 in Figure 3-26).

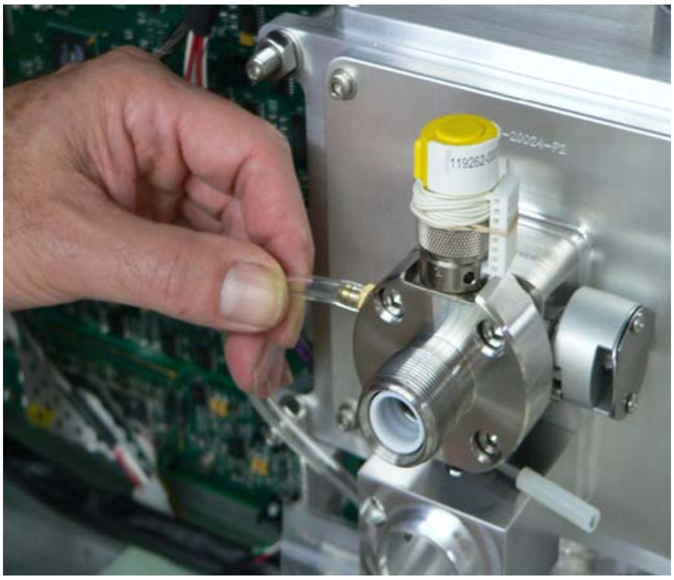


Figure 3-28. Removing the foreline hose from its connection

e. Remove the four screws holding the vacuum manifold probe plate (Figure 3-29 and item 10 in Figure 3-26 on page 3-35). Support the plate with your hand as shown in Figure 3-29. Arrows point to the four hex screw locations (items 1–4).

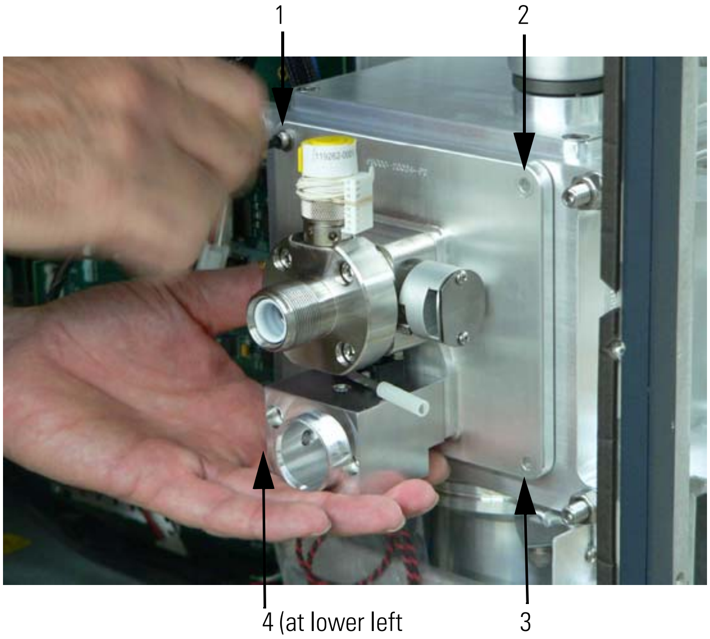


Figure 3-29. Unscrewing the vacuum manifold probe plate

f. Remove the vacuum manifold probe plate (Figure 3-30).

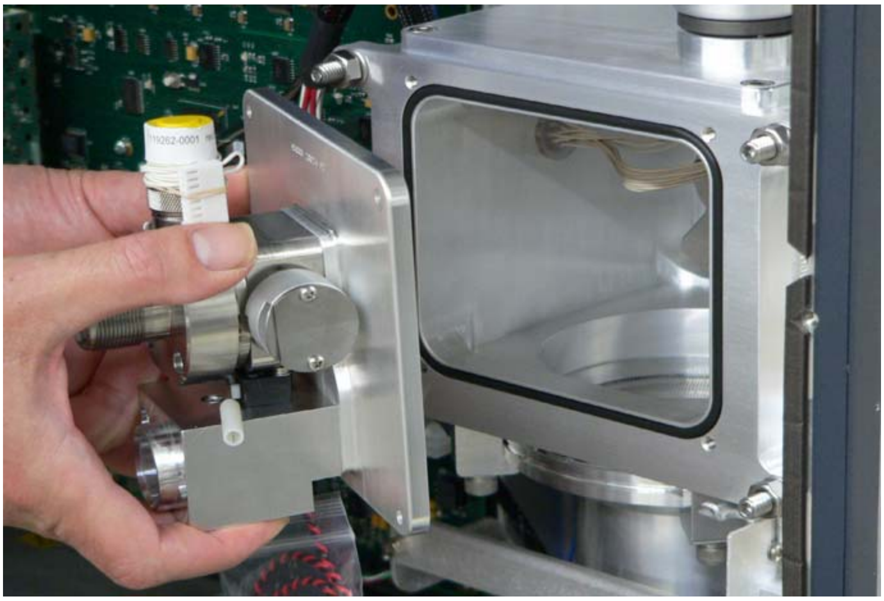
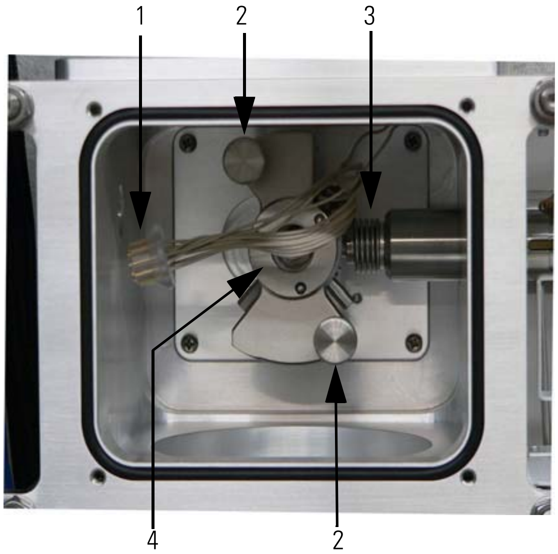


Figure 3-30. Removing the vacuum manifold probe plate

g. Unplug the 12 pin feedthrough harness from the feedthrough (Figure 3-31).



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

Figure 3-31. Interior of vacuum manifold

h. Remove the ion source assembly from the vacuum manifold (Figure 3-32) by first loosening the ion source thumbscrews (item 2 in Figure 3-31).

i. Second, as you remove the ion source assembly (item 1 in Figure 3-32) gently shift it to the left (arrow 2 in Figure 3-32) before and while pulling it out. This will allow the ion source assembly to disengage from the transfer line bellows (item 3 in Figure 3-32) as it is removed. Alternatively, gently depress the transfer line bellows (Figure 3-31) to disengage it from the ion source assembly.

The ion source assembly is held together with a clip (item 8 in Figure 3-33). 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 3-33) and the back of the magnet yoke (item 3 in Figure 3-33) when you handle the ion source assembly. This prevents unsecured components inside of the ceramic lens holder from falling out.

Caution When handling the ion source assembly, it is important to handle it with gentle finger pressure on each end (as instructed above) to keep unsecured components from falling out of the assembly. ▲

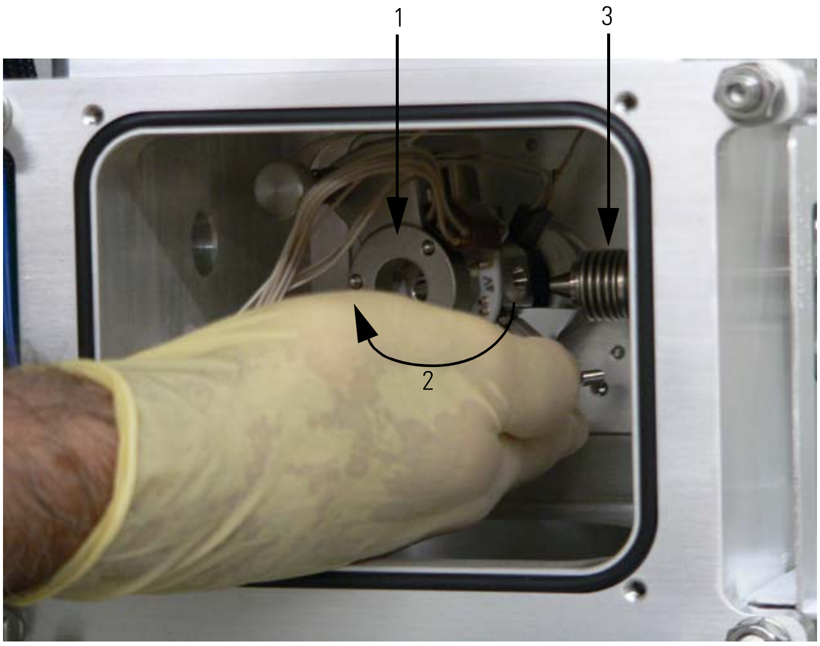
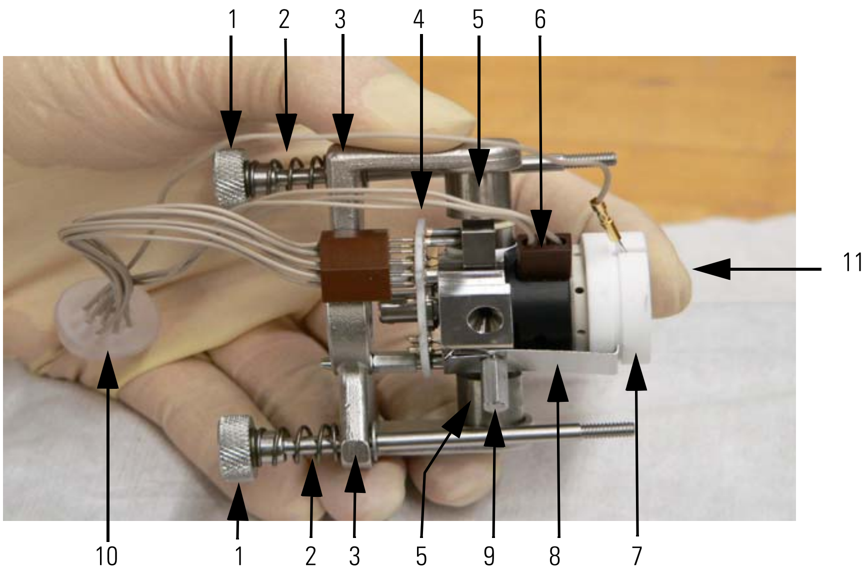


Figure 3-32. Removing the ion source assembly from the vacuum manifold*

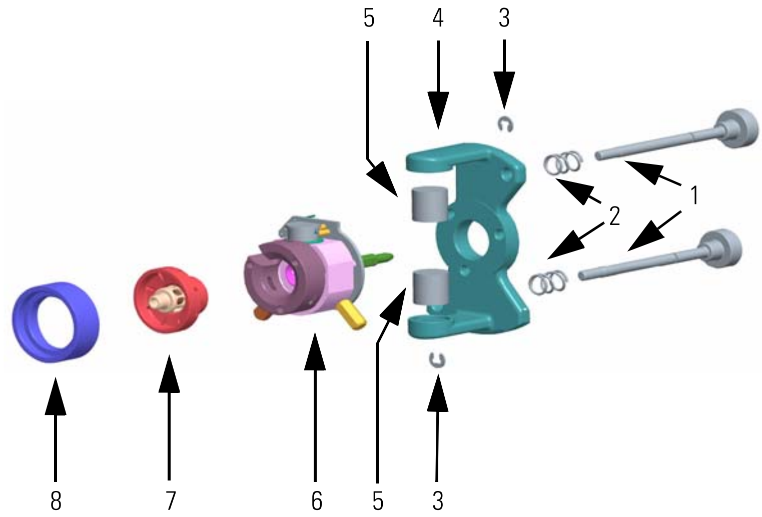
*The ion source assembly (item 1) is gently shifted to the left (arrow 2) to allow the ion source assembly to disengage from the transfer line bellows (item 3) as it is removed.



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 3-33. Ion source assembly

An exploded view of the ion source assembly is shown in Figure 3-34.



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 3-34. 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 3-34).

5. Clean the ion source lens assembly according to the procedure in topic "Cleaning Stainless Steel Parts" on page 3-15. 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 topic "Starting Up the System after a Shutdown" on page 2-9.

Cleaning the Ion Source

If cleaning the ion volume and ion source lens assembly does not restore system performance, you might need to clean the ion source. Clean the ion source 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, do the following:

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 LTQ Orbitrap XL ETD. (See topic "Shutting Down the LTQ Orbitrap XL ETD Completely" on page 2-7.)

Caution Shut down and unplug the LTQ Orbitrap XL ETD before proceeding with the next steps of this procedure. ▲

   c. Remove the ion source assembly by following the procedures in step 2 in topic "Cleaning the Ion Source Lens Assembly" on page 3-34.

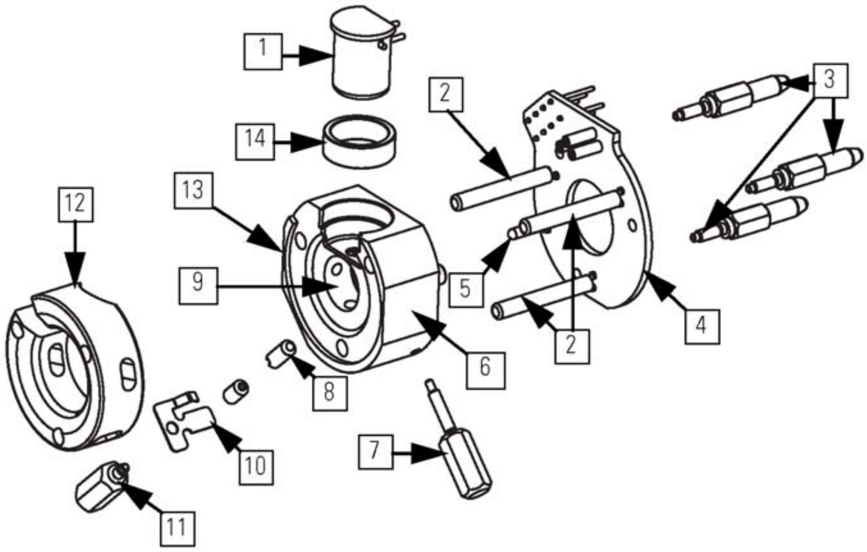
Note Wear clean, lint- and powder- free gloves when you handle parts inside the vacuum manifold. ▲

2. Disassemble the ion source assembly (Figure 3-33 and Figure 3-34), remove and disassemble the ion source (Figure 3-35).

   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 3-35. Ion source, exploded view

d. Remove the three base studs (item 3 in Figure 3-35). Be careful not to damage the leads on the Ion Source PCB (item 4 in Figure 3-35).

e. Gently remove the Ion Source PCB (item 4 in Figure 3-35) from the ion source by loosening the spring clip thumbscrew (item 11 in Figure 3-35) and the spring clip (item 10 in Figure 3-35) and sliding the three cartridge heaters and the temperature sensor (items 2 and 5 in Figure 3-35) off the ion source and pulling the filament (item 1 in Figure 3-35) straight away from the three filament connectors on the Ion Source PCB (item 4 in Figure 3-35). Do not bend or twist the cartridge heaters or temperature sensor.

f. Remove the filament and ceramic spacer (items 15 and 1 in Figure 3-35) from the ion source block (item 6 in Figure 3-35).

g. Remove the ion volume key thumbscrew (item 7 in Figure 3-35).

Note It is not necessary to remove the ion volume pin (item 8 in Figure 3-35). If you remove it, you should reinsert it just far enough so the ball will keep an ion volume (item 9 in Figure 3-35) 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 topic "Cleaning Stainless Steel Parts" on page 3-15 and "Cleaning Non-Stainless Steel or Hybrid Parts" on page 3-17.

    b. Reassemble the ion source block.

    c. Reassemble the ion source assembly.

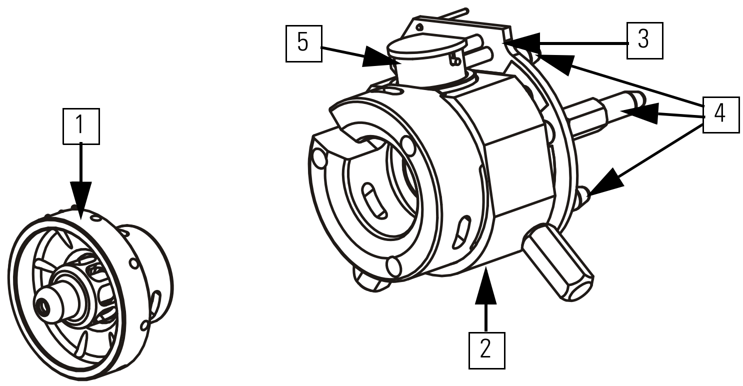
    d. Reinstall the ion source assembly into the vacuum manifold by following step 2 of topic "Cleaning the Ion Source Lens Assembly" on page 3-34 in reverse order.

4. Restore the ETD Module to operational status. See topic "Starting Up the System after a Shutdown" on page 2-9.

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 3-36.



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

Figure 3-36. Ion source lens assembly and ion source

Supplies needed for replacing the ion source filament:

- Filament Assembly DSQ II (P/N 120320-0030)
- Gloves, clean, lint-free, and powder-free
- Lint-free cloth

To replace the ion source filament, do the following:

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 LTQ Orbitrap XL ETD. (See topic "Shutting Down the LTQ Orbitrap XL ETD Completely" on page 2-7.)

Caution Shut down and unplug the LTQ Orbitrap XL ETD before proceeding with the next steps of this procedure. ▲

    c. Remove the ion source assembly by following the procedures in step 2 in topic "Cleaning the Ion Source Lens Assembly" on page 3-34.

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

2. Disassemble the ion source assembly (Figure 3-33 and Figure 3-34), remove and disassemble the ion source (Figure 3-35).

    a. Remove the ion source lens assembly (item 1 in Figure 3-36).

    b. Remove the three base-studs (item 3 in Figure 3-35, item 4 in Figure 3-36).

    c. Remove the filament assembly (items 1 and 15 in Figure 3-35, item 5 in Figure 3-36) and ion source block (item 2 in Figure 3-36) from the three filament connectors and cartridge heaters (item 2 in Figure 3-35) on the Ion Source PCB (item 4 in Figure 3-35) according to the procedure in step e of topic "Cleaning the Ion Source" on page 3-42 .

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

3. Inspect and install a new filament assembly:

   a. Verify that the filament wire is centered in the electron lens hole. Figure 3-37 shows the centered filament wire as seen from the bottom of the filament through the electron lens hole.

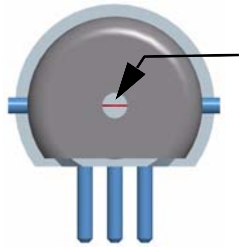


Figure 3-37. Filament wire as seen from the bottom of the filament through the electron lens hole

   b. Insert the filament into the ceramic spacer of the ion source block (item 14 in Figure 3-35).

   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 3-35, item 4 in Figure 3-36).

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 topic "Starting Up the System after a Shutdown" on page 2-9.

Note 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

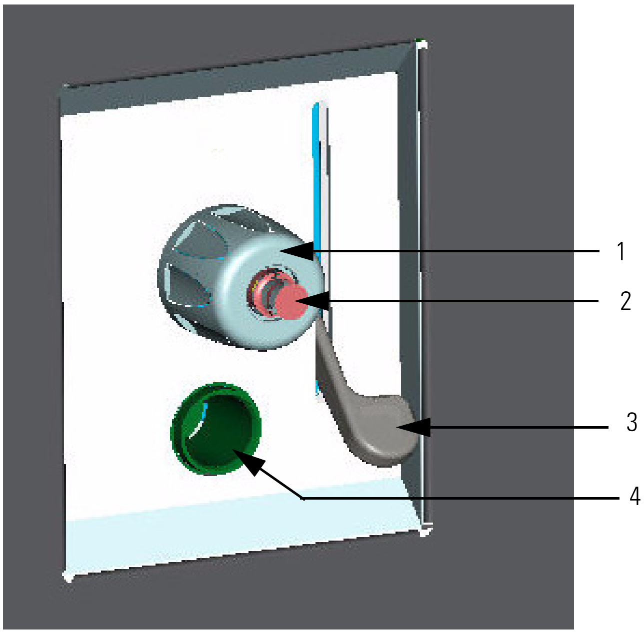
This topic provides the procedure for replacing inlet valve components. Perform this procedure when the inlet valve seal or the inlet valve is being replaced.

Tools and supplies needed for replacing inlet valve components:

- Ball Valve, complete (P/N A0101-02530)
- Inlet Valve Seal Kit (P/N 119265-0003)
- Lint-free cloth
- Replacement Ball Valve O-ring and Seal Kit (P/N 76461-2002)
- Wrench, open-ended, 5/16-in
- Wrench, Allen, 4 mm

To replace inlet valve components, do the following:

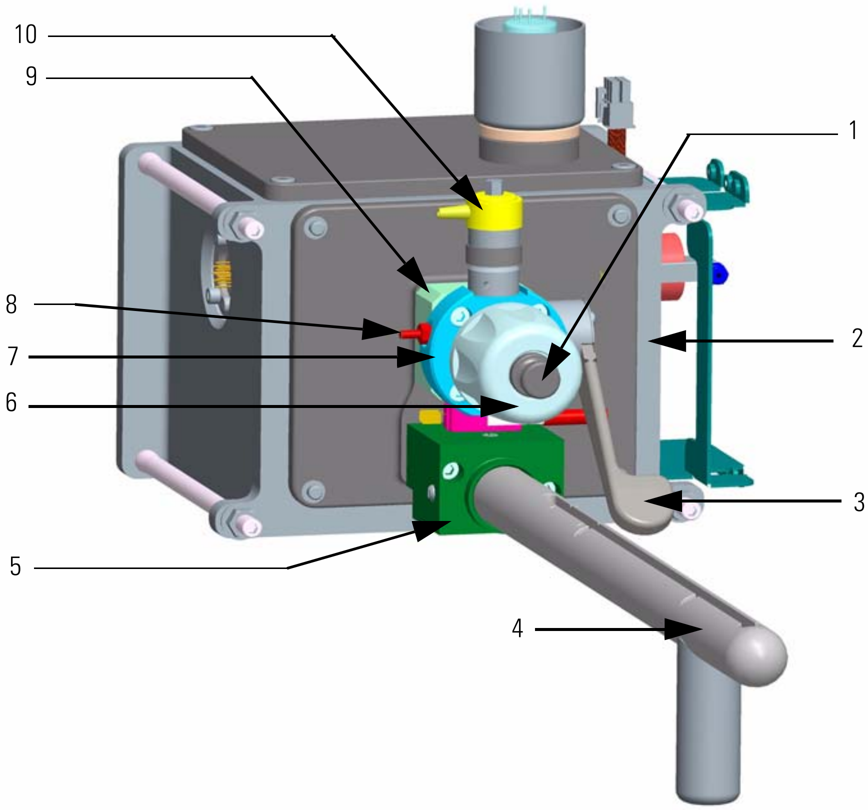
1. Close the inlet valve by pulling the inlet valve lever down (Figure 3-38).



Labeled components: 1=inlet valve knob, 2=inlet valve plug, 3=inlet valve lever in the down (closed) position, 4=guide bar opening

Figure 3-38. Inlet valve

2. Remove the inlet valve knob, plug, and ferrule (Figure 3-39).



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=ball valve housing, 10=inlet valve solenoid

Figure 3-39. Inlet valve components (ion volume tool not shown)

3. Remove the existing inlet valve seal.

   a. Insert the inlet valve seal removal tool (Figure 3-40) into the inlet valve.

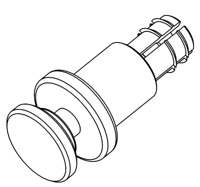


Figure 3-40. Inlet valve seal removal tool (P/N 119283-0001)

   b. Press the button on the tool to engage the seal.

   c. Pull out the seal and discard it.

4. Replace the inlet valve seal with a new one.

5. Put ferrule, knob, and plug back into the inlet valve opening.

Caution Do not scratch the surface of the seal. Use the supplied tool only. ▲

Changing 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 LTQ Orbitrap XL ETD be placed in Service mode after the vials have cooled. (Vial cooling is done in Off condition.) Refer to the following sections for procedures to be used to change the reagent vials:

- "Place the Instrument in Off Condition and Service Mode" on page 3-49
- "Removing the ETD Main Access Panel" on page 3-52
- "Install/Exchange the Reagent Vials" on page 3-53

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. Prevent this from occurring by removing and replacing the ETD reagent vials only when they are empty.

Caution To preserve the integrity of the ETD reagent vial septums, remove and replace the ETD reagent vials only when they are empty. Do not reinstall used vials. ▲

Note 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). ▲

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

Place the Instrument in Off Condition and Service Mode

The power switches control power to the LTQ Orbitrap XL ETD (MS and ETD Module). The ETD Module power switches control the power to the ETD Module only. When the LTQ Orbitrap XL ETD 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.

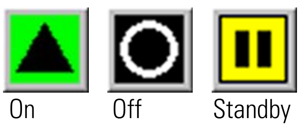
Normally, the ETD Module Power and Service switches remain On. Use the FT Electronics switch on the MS unit to place the LTQ Orbitrap XL ETD in Service mode. Turn On and Off the instrument (both ETD Module and MS) with the MS Main Power switch.

Warning 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). Do not attempt to replace reagent vials or to service heated components until you have determined that they have cooled to a safe temperature for handling. ▲

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

To place the LTQ Orbitrap XL ETD in Off Condition and Service mode and to verify that the vials are safe to handle, do the following:

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 3-9 on page 3-20.)

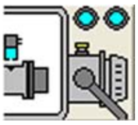


   You can determine the state of the MS detector by observing the state of the On/Standby button on the Control/Scan Mode toolbar. The three different states of the On/Standby button are shown at the left.

2. Choose **Control > Off** from the Tune Plus pull-down menu to place the system in Off condition. When the MS detector is in Off

condition, the LTQ Orbitrap XL ETD turns off the ion source sheath gas, auxiliary gas, high voltage, and all of the ETD Module heaters.

Note It is important to choose **Control > Off** from the Tune Plus pull-down menu in order 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 3-41).

   Observe the temperature of Vial 1 in the Actual column of the Reagent Ion Source dialog box (Figure 3-41). Nitrogen cooling gas will flow until the vial reaches 70 °C. (See topic "Turning Off the Reagent Ion Source: What to Expect" on page 2-14.) Allow up to 90 minutes for the vial temperature to reach ambient temperature (about 30 °C).

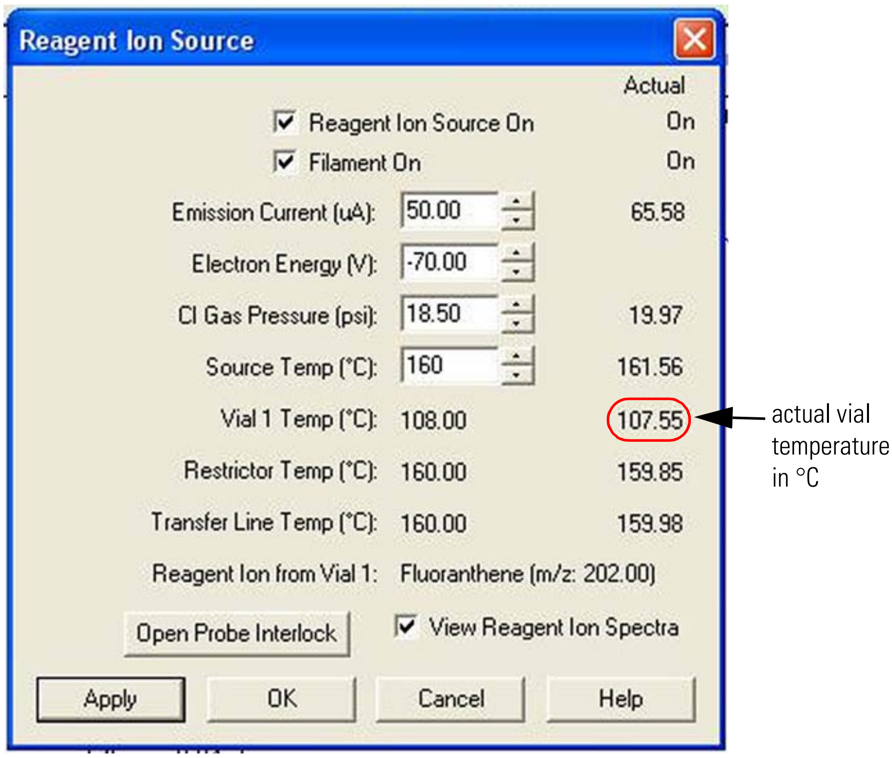


Figure 3-41. Reagent Ion Source dialog box

Warning Do not attempt 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.
Allow the vials to cool to about 30 °C (allow up to 90 minutes after the cooling gas stops) before proceeding 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 turbopumps and the forepumps in both the mass spectrometer and the ETD Module.

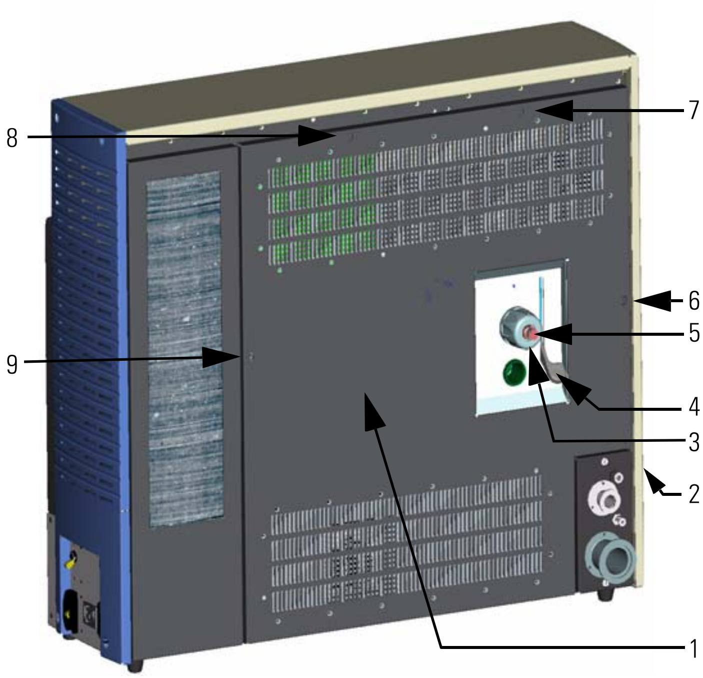
Note Do not place the ETD Module Service switch into its Service mode (Off) position while the MS switches are left in their On positions. This could cause communication problems between the MS and the ETD Module. The ability to control the Service mode for both the MS and the ETD Module at one point (at the FT Electronics switch) is a safety feature. ▲

Warning Do not place the system in Service mode until the vials reach a safe temperature (about 30 °C). System temperature monitoring will stop when the system is placed in Service mode. Do not attempt to handle the vials, the vial holders, or the heater assembly until a safe temperature is reached (about 30 °C). ▲

The LTQ Orbitrap XL ETD is now in Service mode and the vials are at a safe temperature for handling.

Removing the ETD Main Access Panel

Figure 3-42 shows a schematical view of the rear side of the ETD Module.



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 3-42. Schematical rear view of the ETD Module

To remove the ETD main access panel, do the following:

1. Place the ETD Module to Service mode as directed in topic "Place the Instrument in Off Condition and Service Mode" on page 3-49.

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

Warning 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 may be too hot to touch. Exercise caution and verify that all of these components are safe to touch before handling them. ▲

Note 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 (ETD forepump) and ETD turbopump will continue operating. ▲

2. Remove the inlet valve lever (item 4 in Figure 3-42 on page 3-52) by pulling it down and away from the ETD Module main access panel.

Caution **Do not rotate the inlet valve lever upwards** (to the open position) without the inlet valve plug (item 5 in Figure 3-42) or the ion volume tool in place. It must remain in its down (closed) position to avoid catastrophic venting of the system. ▲

3. Remove the inlet valve knob (item 3 in Figure 3-42) and the inlet valve plug (item 5) by unscrewing the inlet valve knob. Be sure that the inlet valve lever (item 4) remains in the down position.

4. Remove the four panel fasteners (items 6, 7, 8, 9 in Figure 3-42).

5. Tilt the top of panel towards you and lift it up and away from the ETD Module.

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

Install/Exchange 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, do the following:

1. Remove the back panel from the ETD Module (see topic "Removing the ETD Main Access Panel" on page 3-52). This exposes the reagent inlet source heating unit, which has its own cover (Figure 3-43 on page 3-54).

Warning Follow the procedures described in topic "Place the Instrument in Off Condition and Service Mode" on page 3-49 before removing the back panel of the ETD Module. 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 attempt to handle the vials before it is safe to do so. ▲

2. Make sure that the vial heater cover is cool to the touch.

Warning The vial heaters can be at 108 °C (or set point). Allow sufficient time for the vials to cool (up to 90 minutes) and then place the system in Service mode. (See topic "Place the Instrument in Off Condition and Service Mode" on page 3-49.) Verify that the vial heater cover is safe to handle before attempting to remove the vial holders and reagent vials. ▲

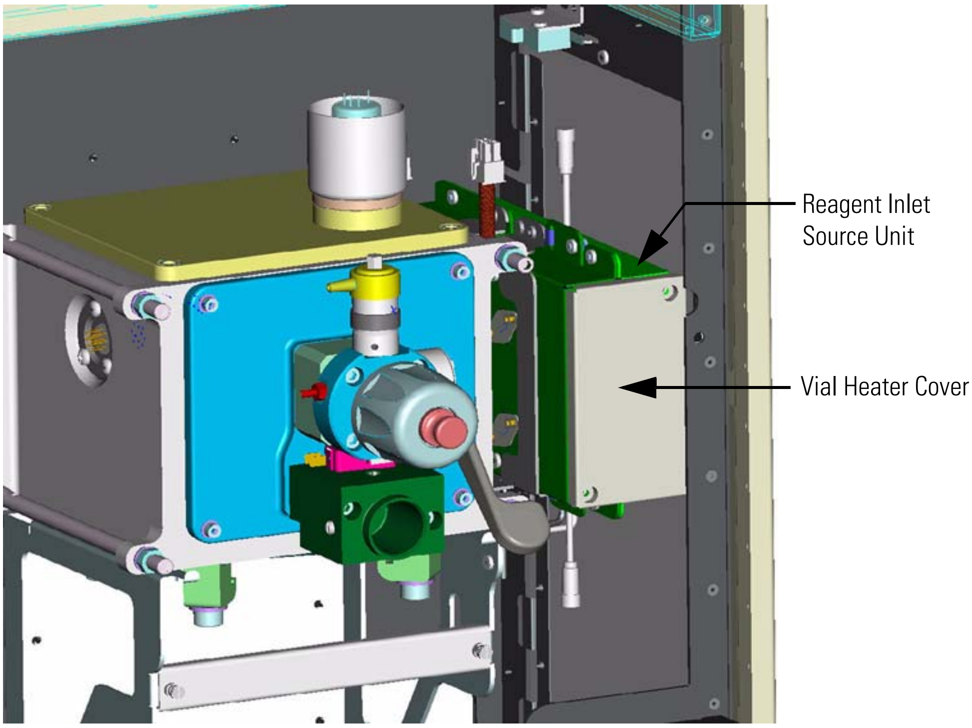


Figure 3-43. ETD Module with back panel removed

3. Remove the vial heater cover. The screws that need to be removed require a 3/32 inch or 2.38 mm hex driver. The vial heater cover is located on the right side of the ETD Module as you view it from the back of the LTQ Orbitrap XL ETD (Figure 3-43).

4. Remove the vial holder by gently pulling it out of the vial heater. 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 3-44. These ribs prevent the vial holder from rotating once it is placed into the vial heater. Figure 3-45 on page 3-56 shows the tab and ribs of a vial holder in the vial heater.

Note Dispose of an empty fluoranthene vial in accordance with its MSDS. ▲

Figure 3-44. Reagent vials with holders

Note Store and handle all chemicals in accordance with standard safety procedures. The Material Safety Data Sheet (MSDS) describing the chemicals being used are to 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). ▲

5. Take a vial containing the ETD reagent (fluoranthene) from its box and place it into a vial holder.

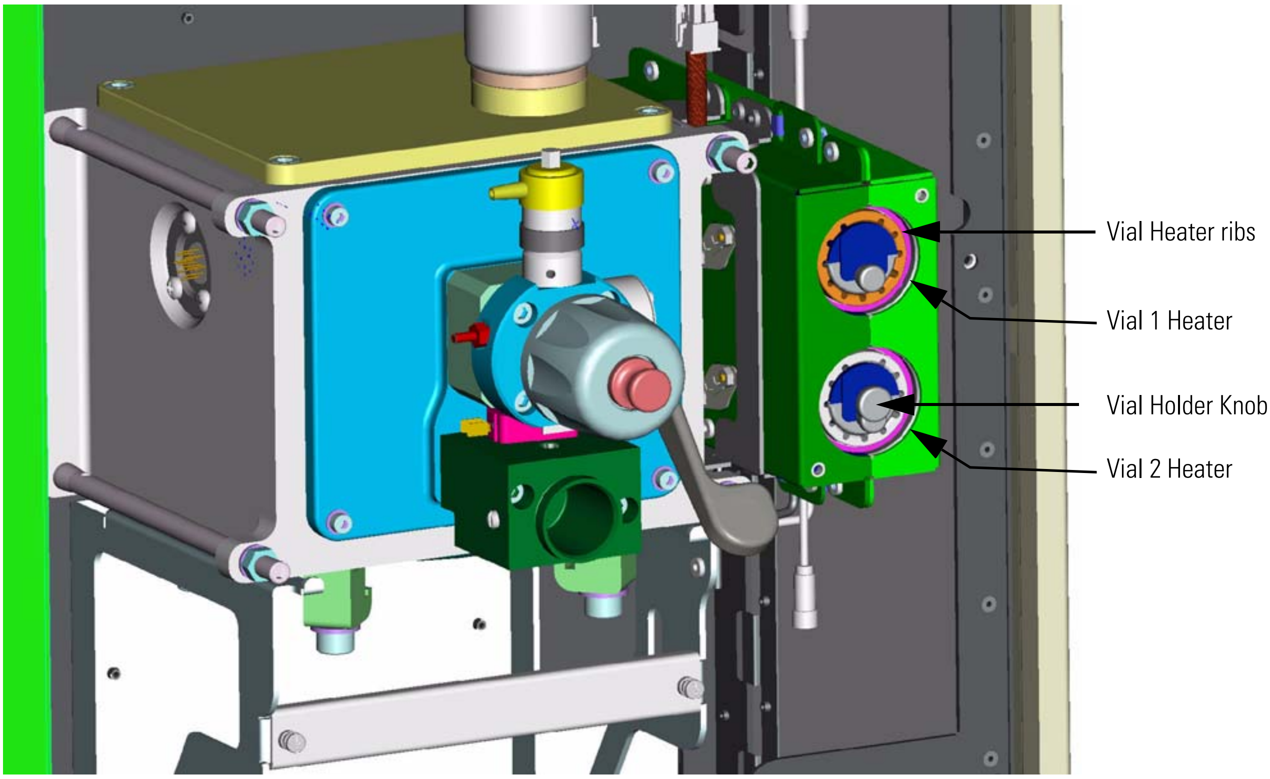


Figure 3-45. ETD Module with vial heater cover removed

6. Place 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.

7. Place the empty vial from the box into the other vial holder if an empty vial is not already installed.

8. Place this empty vial and its vial holder into the Vial 2 heater (bottom vial heater) if an empty vial is not already installed.

Warning 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 containing the reagent may escape to the laboratory causing a safety problem.
- The ETD Module will not operate correctly and the filament will burn out. ▲

9. Replace the vial heater cover over the vial heaters.

10. Reinstall the back panel of the ETD Module. See topic "Removing the ETD Main Access Panel" on page 3-52. The ETD Module will not turn on unless the back panel is installed.

11. Start the system:

    a. Toggle the FT Electronics switch to the On position.

       The system will boot to Standby mode. Then ion source heater, flow restrictor, and transfer line heaters will start heating. Monitor these temperatures in the Status View on the right side of the Tune Plus window. (See Figure 3-9 on page 3-20.) 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, flow restrictor, and transfer line heaters are at their operating temperatures. (See Figure 3-41 on page 3-50.)

The LTQ Orbitrap XL ETD is now ready for use.

Changing the Reagent Ion Source Flow Restrictors

To change the reagent ion source flow restrictors, do the following:

1. Shut down completely the instrument according to the procedures in topic "Shutting Down the LTQ Orbitrap XL ETD Completely" on page 2-7.

Warning 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 may be too hot to touch. Verify that all of these components are safe to touch before handling them. ▲

2. Remove the ETD side access panel according to the instructions in topic "Removing the ETD Side Access Panel" on page 3-33.

Caution 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. ▲

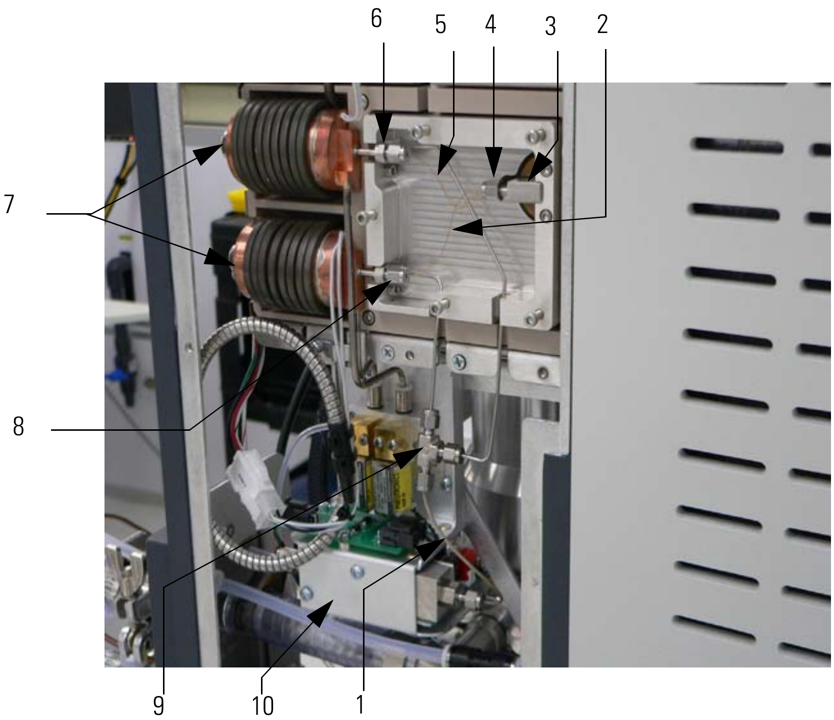
3. Remove the four screws that hold the reagent inlet cover in place.

Warning The reagent inlet cover may be too hot to touch. Verify that the reagent inlet cover is at or near room temperature before handling it. ▲

4. Remove the five screws that hold the restrictor oven cover in place.

Warning The restrictor oven cover may be too hot to touch. Verify that the restrictor oven cover is at or near room temperature before handling it. ▲

5. Replace both fused silica restrictors and their ferrules by removing their Swagelok® nuts. See Figure 3-46.



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 3-46. Reagent inlet assembly

6. Thread two pieces of fused silica tubing (P/N 98000-20060) into the two hole ferrule (P/N 00101-08-00006) from the Installation Kit for the Reagent Inlet Module (P/N 98000-62006). 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 3-46) 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 3-46) and tighten the Swagelok fitting.

Caution Do not overtighten the ferrules. The ferrules may loosen after they are first heated. If this occurs retighten them if necessary. ▲

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 3-46) to the Tee below the reagent inlet assembly (item 9 in Figure 3-46) and from the gas valves (item 10 in Figure 3-46).

13. Replace the old PEEKsil tubing with new PEEKsil tubing (P/N 00109-02-00020) from the Installation Kit for the Reagent Inlet Module (P/N 98000-62006).

14. Close the ETD Module and restart the instrument. Follow the procedures given in topic "Starting Up the System after a Shutdown" on page 2-9.

Cleaning the Fan Filters of the ETD Module

You need to clean the fan filters every four months. The fan filters are located at the rear of the ETD Module on the left side (as viewed from the back of the ETD Module). See Figure 3-47.

Figure 3-47. ETD Module, top panel

To clean the fan filters of the ETD Module, do the following:

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 allow them to air dry.

5. Reinstall the fan filter in the fan filter bracket.

Maintenance of the Recirculating Chiller

For the NESLAB ThermoFlex™ 900 recirculating chiller, the checks described in this section should be carried out on a regular basis.

Note 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. Replacement frequency depends on the operating environment and amount of usage.

Warning Before changing the operating fluid make sure it is at safe handling temperature. ▲

Fluid Bag Filter

The ThermoFlex 900 recirculating chiller 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.

Chapter 4 Replaceable Parts

This chapter contains part numbers for replaceable and consumable parts for the MS detector, data system, and kits. To ensure proper results in servicing the LTQ Orbitrap XL ETD system, order only the parts listed or their equivalent.

For information on how to order parts, refer to the topic "Customer Support" in the *LTQ Orbitrap XL / LTQ Orbitrap Discovery Preinstallation Requirements Guide*.

Note Not all parts are available for purchase separately. Some parts may only be available for purchase as part of a kit or assembly. ▲

This chapter contains the following topics:

Parts List for the Mass Analyzer

This topic contains parts lists for the mass analyzer portion of the LTQ Orbitrap XL ETD.

Table 4-1. Parts for the LTQ Orbitrap XL

Designation	Part No.
LTQ Orbitrap XL; 50 Hz*	072 3852
LTQ Orbitrap XL; 60 Hz	072 3862
Edwards Pumps kit, for LTQ-Hybrid	121 6450
Pumps kit 2, Orbitrap (ILMVAC)	121 4310
ESI probe, for Ion Max source	OPTON-20011
Nanospray II Ion Source†	OPTON-20050
Static Nanospray†	OPTON-20051
Dynamic Nanospray†	OPTON-97017
APCI probe†	OPTON-20012
APPI probe†	OPTON-20026

*Module, for parts list see below.

†Optional equipment.

Table 4-2. Parts LTQ Orbitrap XL; 50 Hz (P/N 072 3852)

Designation	Part No.
Basic system Orbitrap-2*	122 4790
LTQ XL Linear trap MS system, with computer	LTQ02-10001
Low flow metal needle for API 2 probes	OPTON-30004
Dell Laserprinter 1700	106 3385
Recirculating chiller Neslab ThermoFlex 900 PD-1 230V/50 Hz	101161010000004
Upgrade kit Orbitrap HCD option*	122 4800

*Module, for parts list see below.

Parts Basic System

This section contains parts lists for the mechanical components of the LTQ Orbitrap XL ETD.

Table 4-3. Parts basic system Orbitrap-2 (P/N 122 4790)

Pos. No.	Qty.	Designation	Part No.
0010	1	Orbitrap-2 chamber; complete*	122 4780
0020	1	Orbitrap-D30; complete	116 5000
0030	1	CLT and lens system; complete	122 1200

Table 4-3. Parts basic system Orbitrap-2 (P/N 122 4790)

Pos. No.	Qty.	Designation	Part No.
0040	1	Pumping system Orbitrap*	118 4490
0050	1	Water supply Orbitrap*	117 8460
0060	1	Orbitrap panels	117 2910
0070	1	Mounting devices Orbitrap-2	117 7891
0080	1	Gas supply Orbitrap-2*	117 7881
0090	1	Orbitrap Installation Kit*	118 8120
0100	1	Electronic parts Orbitrap-2*	800 1110

*Module, for parts list see below.

Table 4-4. Parts Upgrade kit Orbitrap HCD option (P/N 122 4800)

Pos. No.	Qty.	Designation	Part No.
0010	1	Collision cell, with mount	122 1320
0020	1	Flange, for options; complete	122 1250
0030	1	Cable kit, Upgrade LTQ Orbitrap XL	122 5100
0040	1	Upgrade kit gas supply LTQ Orbitrap XL*	122 4820
0050	1	Cable, power distribution/valve	210 0310

*Module, for parts list see below.

Table 4-5. Parts Orbitrap Installation Kit (P/N 118 8120)

Pos. No.	Qty.	Designation	Part No.
0010	1	Orbitrap Installation Kit Ilmvac	1196990
0020	4	One ear clamp; Ø 17.5	114 4910
0030	6	Ferrule, 1/16”, for GVF/16	067 4800
0040	3.0 m*	Tube, 1/8" × 2.1- 1.4301	026 1000
0050	3.0 m*	Hose; 4 x 1, Teflon	069 0280
0060	6	Clamping piece 8/16	037 0130
0070	1	Contact wrist strap, with coiled cord	119 3050
0080	1	Ferrule, stainless steel; R. 1/8"	052 0950
0090	1	Ferrule, stainless steel; V. 1/8"	052 2520
0100	1	Cap nut, stainless steel; 1/8”	052 0890
0110	1	Connector; C19 to C14	082-2528
0120	10	Miniature fuse; 5 x 20 mm, 8 A	201 1850

*Specify desired length.

Parts Orbitrap Analyzer

Table 4-6. Parts Orbitrap-2 chamber; complete (P/N 122 4780)

Pos. No.	Qty.	Designation	Part No.
0010	1	UHV chamber; complete	116 6110
0020	1	Vacuum chamber, complete	116 6131
0040	4	Washer; 8.4×15×1.5, stainless steel	047 0860
0050	4	Screw; M8×25, silver plated	119 1210
0060	4	Pan head screw; M 2 x 8 DIN 84 A4	045 0720
0070	2	Screw cyl. M 4 x 12 DIN912	045 2800

Parts Pumping System Orbitrap

Table 4-7. Parts pumping system Orbitrap (P/N 118 4490)*

Pos. No.	Qty.	Designation	Part No.
0010	1	Turbomolecular pump TMU262; modified	118 4340
0020	2	Turbomolecular pump; TMH 071 P	114 1500
0040	1	Water cooling for TMH 262	114 9140
0050	5	Water cooling for TMH 071 P	079 4742
0080	1	UHV gauge IKR 270; short	118 1380
0130	1	Compact Pirani Gauge TPR280	115 6400

*For a schematical overview of the vacuum system, refer to Figure 1-20 on page 1-28.

Two kits are available for the pumping system, comprising either pumps, gauges, and cooling (pump kit Orbitrap: P/N 117 5000) or hoses, clamps, and gaskets (pump system Orbitrap: P/N 117 5010):

Table 4-8. Parts pump kit Orbitrap (P/N 117 5000)

Pos. No.	Qty.	Designation	Part No.
0010	1	Turbomolecular pump TMU262; modified	118 4340
0020	2	Turbomolecular pump; TMH 071 P	114 1500
0030	1	UHV gauge IKR 270; short	118 1380
0040	1	Compact Pirani Gauge TPR280	115 6400
0050	1	Water cooling for TMH 262	114 9140
0060	5	Water cooling for TMH 071 P	079 4742
0070	1	PVC hose, with steel helix; ID=45 mm, L=1.6 m	118 4330
0080	2	Hose nipple, DN 40, ISO-KF-45	115 9230
0090	1	Venting flange; DN 10, KF-G1/8"	118 4400

Table 4-8. Parts pump kit Orbitrap (P/N 117 5000), continued

Pos. No.	Qty.	Designation	Part No.
0100	1	Splinter shield for turbopumps, with DN 100 CF-F flange	119 8590
0110	2	Centering ring, with integrated splinter shield; DN 63 ISO	119 8600

Table 4-9. Parts pump system Orbitrap (P/N 117 5010)

Pos. No.	Qty.	Designation	Part No.
0010	2	Gasket; NW 100 CF, copper	055 2440
0020	1	Hose, metal; KF16-KF25 - 250mm	115 4130
0030	1	Gasket; copper, NW 35	055 0480
0040	2	Metal tube, KF NW16×250	052 4260
0050	2	KF Tee piece; NW 16 KF, stainless steel	052 4230
0060	8	Centering ring with o-ring; DN 16, Viton	052 2140
0070	1	Centering ring with o-ring; DN 25, Viton	052 2150
0080	1	Centering ring; NW 16/10, aluminum-Viton	052 2200
0090	6	Clamping ring; NW 10/16, KF	052 1830
0100	1	Clamping ring; NW 20/25, KF	052 1560
0110	1	Reducing cross piece; DN40/DN16 KF	118 4310
0120	1	Metal tube; DN40x500	118 4350
0130	1	Metal tube; DN40x750	118 1290
0140	2	Hose clamp; NW 40	118 1320
0150	4	Centering ring; NW 40 KF, aluminum-Viton	052 2260
0160	4	Tension ring; NW 32/40 KF	118 1250
0170	8	Clamping screw; DN63-100 ISO, aluminum	104 2670
0180	1	Blank flange; NW 16 KF, aluminum	118 1300

Parts Gas and Water Supply

This topic contains parts lists for the gas and water supply of the LTQ Orbitrap XL ETD. For a schematical overview of the gas supply, refer to Figure 1-26 on page 1-36.

Table 4-10. Parts gas supply (P/N 117 7881)

Pos. No.	Qty.	Designation	Part No.
0010	2	Bulkhead union; 1/16”, for hose 4 x 1 (for P/N 069 1130)	115 3660
0020	1	Bulkhead union; 1/8"×1/8"	052 3450
0030	4.5 m*	Hose; 4 x 1, Teflon	069 0280
0040	3.5 m*	Hose; 4 x 1, polyurethane, blue	069 1130

Table 4-10. Parts gas supply (P/N 117 7881)

Pos. No.	Qty.	Designation	Part No.
0050	0.5 m*	Capillary 1/16" ID-SS	060 5470
0060	2	Plug-in T-piece; 3 x 6mm	112 8140
0070	1	Stainless steel reducing union; Swagelok, 6 mm-1/16”	117 8070
0080	1	T-piece; 1/16" (SS-100-3)	052 3550
0090	1	Coupling; 1/16”, SS-100-6	052 4340
0100	3	PEEKSIL capillary; 1/16", 500 × 0.075 mm	118 6970
0110	1	Reducer Swagelok; 1/8" × 1/16", stainless steel	066 2880
0120	2	Support jack; for hose 4 mm	104 9620
0130	6	Ferrule; 1/16" GVF/16	067 4800
0140	1	N_2 venting Orbitrap	119 1480
0150	1	Connector 1/8”, for hose OD 4 mm	112 8680
0160	1	Cap nut; 1/16”, stainless steel	052 0880
0170	3.0 m*	Hose; 2 x 1, PTFE	109 1650
0180	1	Sleeve; Ø 6 mm	104 7320

*Specify required length.

Table 4-11. Upgrade kit gas supply LTQ Orbitrap XL (P/N 122 4820)

Pos. No.	Qty.	Designation	Part No.
0050	0.10 m*	Capillary 1/16" ID-SS	060 5470
0070	1	Stainless steel reducing union; Swagelok, 6 mm-1/16”	117 8070
0080	1	T-piece; 1/16" (SS-100-3)	052 3550
0090	1	Coupling; 1/16”, SS-100-6	052 4340
0100	2	PEEKSIL capillary; 1/16", 500 × 0.075 mm	118 6970
0130	6	Ferrule; 1/16" GVF/16	067 4800
0190	2	Capillary; PEEKsil, 1/16", 0.1 × 500 mm	122 3420
0200	1	Valve, with angle	122 4070

*Specify required length.

Table 4-12. Parts water supply (P/N 117 8460) *

Pos. No.	Qty.	Designation	Part No.
0010	2	Quick coupling insert; 9.6 mm	114 1640
0020	2	Quick coupling body; 9.6 mm	113 8960
0030	10 m†	Hose; 9 x 3, black, PVC	104 9540
0040	4	Hose clamp; 1-ear, 14.6–16.8 mm	114 4910
0050	1.5 m†	Hose; 4 x 1, Teflon	069 0280

Table 4-12. Parts water supply (P/N 117 8460), continued*

Pos. No.	Qty.	Designation	Part No.
0060	2	Quick coupling insert; Delrin Acetal, NW 6.4	118 5030
0070	2	Quick coupling body; Delrin Acetal, NW 6.4	118 5020
0080	16	Clamping piece 8/16	037 0130
0090	2	Adaptor hose nipple; male, 1/2 x 10	118 5840
0100	1	Flow control sensor	119 1740

*For a schematical overview of the cooling water circuit, refer to Figure 1-30 on page 1-40.

†Specify required length.

Table 4-13. Kit gas-water assembly (P/N 208 7351)

Pos. No.	Qty.	Designation	Part No.
0010	1	Bulkhead union; 1/16”, for hose 4 x 1 (for P/N 069 1130)	115 3660
0020	1	Bulkhead union; 1/8"×1/8"	052 3450
0030	5.0 m*	Hose; 4 x 1, Teflon	069 0280
0040	3.5 m*	Hose; 4 x 1, polyurethane, blue	069 1130
0050	3.5 m*	Capillary 1/16" ID-SS	060 5470
0060	1	Stainless steel reducer, 1/16" OD - 1/8" ID	066 2880
0070	2	Quick coupling insert; 9.6 mm	114 1640
0080	2	Quick coupling body; 9.6 mm	113 8960
0090	6.0 m*	Hose; 9 x 3, black, PVC	104 9540
0100	2	Hose clamp; 1-ear, 14.6–16.8 mm	114 4910

*Specify required length.

Electronic Parts

This section contains parts list for the electronic components of the LTQ Orbitrap XL ETD.

Table 4-14. Electronic parts Orbitrap-2 (P/N 800 1110)

Pos. No.	Qty.	Designation	Part No.
0050	1	Orbitrap-2 Electronics; right panel*	210 1480
0060	1	Orbitrap-2 Electronics; left panel*	208 1020
0070	1	Electronics analyzer Orbitrap-2*	210 0160
0080	1	Electronics main supply Orbitrap*	208 1040
0090	1	Electronics rear panel assembly Orbitrap-2	208 1050
0100	1	Cable kit Orbitrap-2	210 1690
0110	1	Cable kit LTQ-Orbitrap grounding	208 1070

Table 4-14. Electronic parts Orbitrap-2 (P/N 800 1110)

Pos. No.	Qty.	Designation	Part No.
0120	1	Kit Orbitrap assembly material	208 1080
0130	1	Subpackage Orbitrap-2 assembly	210 1660
0140	1	Kit gas-water assembly†	208 7351

*Module, for parts list see below.

†Module, see Table 4-13 on page 4-7.

Electronics – Right Panel

The following replaceable parts are available for the electronics at the right panel of the LTQ Orbitrap XL ETD.

Table 4-15. Parts Orbitrap-2 electronics; right panel (P/N 210 1480)

Pos. No.	Qty.	Designation	Part No.
0010	1	Power supply 1	205 5810
0020	1	Power supply 29V/2A	206 4040
0030	1	Power distribution	206 2130
0040	1	Unit PS 24V/20A	208 1130
0050	1	Unit PS +/-15V/2.75A	208 1140
0060	1	KIT E_RIGHT PANEL ASSEMBLY	206 9790
0070	1	Unit data acquisition*	206 4132
0080	1	Instrument control board	205 4221
0085	1	CLT RF TRIGGER board	208 5880
0090	1	LT ANALOG INTERFACE board Orbitrap-2	208 1940
0100	1	LT DIGITAL INTERFACE board	208 7180
0110	1	UNIT PS-BASIC LOAD	208 5900

*Module, for parts list see below.

Table 4-16. Parts Unit data acquisition (P/N 206 4132)

Pos. No.	Qty.	Designation	Part No.
0010	1	Housing PC2 FTMS / ORBITRAP	115 5320
0020	1	Network interface card LCS 8038 TXR	208 2140
0030	1	MATRIX-STL FRONTEND-PC LTQ-FT	207 6470
0040	1	UNIT_PC POWER SUPPLY PS_ON	209 5950
0050	1	LP DAQ DIGITAL PCI BOARD	206 0501
0060	1	IDC/26POL/1.1M	203 0340
0070	1	DAQ ANALOG FRONT END	206 4150
0080	3	SMB BU-90ø/ST-0ø/0.7M	205 9630

Table 4-16. Parts Unit data acquisition (P/N 206 4132), continued

Pos. No.	Qty.	Designation	Part No.
0090	1	IDC/14POL/0.12M	206 3790
0100	2	IDC/40POL/0.10M	205 2190
0110	1	PS2/DAQ ANALOG	205 9710
0120	1	POWER SUPPLY 2	206 1440
0130	1	Load resistor 4R7	206 5230
0140	1	Angle bracket, for PC	121 8680

Electronics – Left Panel

The following replaceable parts are available for the electronics at the left panel of the LTQ Orbitrap XL ETD.

Table 4-17. Parts Orbitrap-2 electronics; left panel (P/N 208 1020)

Pos. No.	Qty.	Designation	Part No.
0010	1	UNIT HIGH VOLTAGE PS	207 7991
0020	1	UNIT CENTRAL ELECTRODE PS	207 9611
0030	1	LP SPI-BUS-TERMINATION	208 1480

Electronics Analyzer

The following replaceable parts are available for the analyzer electronics of the LTQ Orbitrap XL ETD.

Table 4-18. Parts electronics analyzer Orbitrap-2 (P/N 210 0160)

Pos. No.	Qty.	Designation	Part No.
0010	1	UNIT CLT RF SUPPLY	207 9581
0020	1	UNIT CENTRAL ELECTRODE PULSER	207 9640
0030	1	UNIT TEMPERATUR CONTROLLER	207 8930
0040	1	UNIT PRE AMPLIFIER	207 8900
0060	1	UNIT ION OPTIC SUPPLY, Orbitrap-2	209 9810

Electronics Main Supply

The following replaceable parts are available for the electronics main supply of the LTQ Orbitrap XL ETD.

Table 4-19. Parts electronics main supply Orbitrap (P/N 208 1040)

Pos. No.	Qty.	Designation	Part No.
0010	1	UNIT SWITCH PANEL	208 1120
0020	1	Mains cable; IEC-CONNECTOR-16A	209 6110
0030	1	Mains cable; MAIN INPUT/LINE FILTER	208 1420
0040	1	KIT BAKEOUT-SWITCHES	207 9040
0050	1	Cable loom, mains supply	208 1110
0070	1	Mains cable; LINE FILTER/MAIN SWITCH	208 1280
0080	1	Mains cable; terminal/LTQ-relay	208 1290
0090	1	Mains cable; POWER DIS./SWITCH PANEL 1	208 1300
0100	1	Mains cable; POWER DIS./SWITCH PANEL 2	208 1310
0110	1	Cable; power distribution/LTQ-relay	208 1320
0120	1	Cable loom, power distribution/bakeout timer	207 9010
0130	1	Unit bakeout timer Orbitrap	208 0960
0140	1	KIT MAINS SUP.ASSEMBLY MAT.	208 1100
0150	1	Cable; BAKEOUT-TIMER/POWER DIS.	208 1470
0160	1	Mains cable; POWER DIS./SOCKET R-PUMP	208 1350
0170	1	Mains cable; LTQ-relay/LTQ-filter	208 9230

Parts Lists for the ETD System

This section contains parts lists for the components of the ETD System of the LTQ Orbitrap XL ETD.

Table 4-20. Parts ETD Option for Orbitrap XL (P/N 072 3890)

Pos. No.	Qty.	Designation	Part No.
0010	1	ETD Upgrade kit for Orbitrap XL*	124 1480
0020	1	Software LTQ Orbitrap XL 2.5.5 DVD	124 4030

*Module, for parts list see below.

Table 4-21. Parts ETD Upgrade kit for Orbitrap XL (P/N 124 1480)

Pos. No.	Qty.	Designation	Part No.
0010	1	Upgrade kit Orbitrap XL to ETD*	124 4690
0020	1	UNIT_CLT RF MAINBOARD	207 9581
0030	1	Packaging ETD	124 7040

*Module, for parts list see below.

Table 4-22. Parts Upgrade kit Orbitrap XL to ETD (P/N 124 4690)

Pos. No.	Qty.	Designation	Part No.
0010	1	ETD-Unit Mechanics*	123 9920
0020	1	Collision cell (axial field) with mount, complete	124 0850
0030	1	Connections; antechamber Orbitrap-3	124 1400
0040	1	Quadrupole Orbitrap, complete	123 9200
0050	1	Mounting parts; ETD*	123 9300
0060	1	ETD housing, complete	123 3750
0070	1	Kit ETD electronics*	210 8880
0080	1	ETD upgrade from LTQ XL*	OPTON-97103
0090	1	Cross beam for ETD frame	117 2210
0100	1	Unit CLT-Offset-Filter	211 0470

*Module, for parts list see below.

Mechanical Parts for ETD System

Table 4-23. ETD unit mechanics (P/N 123 9920)

Pos. No.	Qty.	Designation	Part No.
1	1	Transfer tube with flatapole for ETD*	121 7000
2	1	Housing HCD/ETD*	123 1780

*Module, for parts list see below.

Table 4-24. Parts for transfer tube with flatapole for ETD (P/N 121 7000)

Pos. No.	Qty.	Designation	Part No.
0010	1	Tube with flatapole for ETD, complete	121 7400
0020	1	Mount 1, for ETD flatapole	121 7130
0030	3	Rubber bumper; 20x15-M6	121 7370
0040	1	Support, for ETD tube	121 7380
0050	4	Washer 6.4; stainless steel	047 0060
0060	2	Allen screw, stainless steel; M6; 20 long	045 3420
0070	1	Counter support, for ETD tube	121 7490
0080	2	Cylindrical Screw ISO4762-M6X12-A4	045 3300
0090	2	Nut, stainless steel; M6	046 0520

Table 4-25. Parts Housing HCD/ETD (P/N 123 1780)

Pos. No.	Qty.	Designation	Part No.
0010	1	Housing HCD/ETD	123 1740
0020	1	Separating plate HCD/ETD	123 1770
0030	6	Screw M 4 x 8 DIN912	104 4420
0040	1	O-ring 129 X 4 A Viton	124 0520
0050	1	Lid HCD/ETD	123 1760
0060	2	Screw-in connector; 1/16”	118 6150
0070	3	Gasket; NW 63 ISO, aluminum/Viton	055 4060
0080	2	Blank flange; stainless steel, NW 63	065 2620
0090	8	Clamping screw; DN63-100, aluminum	102 8380
0100	4	Washer 8.4; stainless steel	047 0070
0110	4	Screw, hexagonal; M 8 x 35, stainless steel	045 4400
0120	4	Washer 8.4 x 11 x 1.5, stainless steel	047 0860
0130	4	Screw M8 x 35; stainless steel	045 4250
0140	1	Centering ring NW 16 Viton	052 2140
0150	1	Feedthrough; 8-fold 1,5kV DN16KF	123 1750
0160	1	O-ring; 118 X 5 A, Viton	116 8240

Table 4-25. Parts Housing HCD/ETD (P/N 123 1780), continued

Pos. No.	Qty.	Designation	Part No.
0170	1	Box f. feedthrough; KF16 / Sub-D9	123 1800
0180	6	Cylindrical Screw ISO4762-M6X12-A4	045 3300
0190	1	Flange clamp; KF16	114 5860
0200	2	Washer, stainless steel, ID 6.4	047 0850
0210	2	Allen screw, stainless steel; M6; 20 long	045 3420
0220	1	Adapter flange	116 8050
0230	4	Clamping screw; DN63-100 ISO, aluminum	104 2670
0240	3	Guide bolt	124 3930
0300	1	Cable set; HCD/ETD box	123 9660
0400	1	Cable set; HCD/ETD feedthrough	123 9670

Table 4-26. Mounting parts ETD (P/N 123 9300)

Pos. No.	Qty.	Designation	Part No.
0010	1	Pfeiffer - Kit for ETD*	124 1510
0020	1	ILMVAC - Kit for ETD*	124 1520
0030	1	Springer - Kit for ETD*	124 1530
0040	1	Mounting parts - Kit for ETD*	124 1540

*Module, for parts list see below.

Table 4-27. Pfeiffer - Kit for ETD (P/N 124 1510)

Pos. No.	Qty.	Designation	Part No.
0010	1	TURBOPUMP TMH 071 P	114 1500
0020	1	Splinter guard, DN_63_ISO	119 8600
0030	1	Water cooling, for TMH 071 P	079 4742

Table 4-28. ILMVAC - Kit for ETD (P/N 124 1520)

Pos. No.	Qty.	Designation	Part No.
0010	2	Metal hose, DN 16 ISO-KF x500	118 1410
0020	3	Centering ring with o-ring; DN 16, Viton	052 2140
0030	2	Clamping ring; NW 10/16, KF	052 1830
0040	1	Hose flange; NW 25 KF	104 2330
0050	2	Centering ring, with o ring; DN 25, Viton	052 2150
0060	2	Clamping ring, DN 25	052 1560
0070	1	Flange, KF16 - hose OD 19	123 9340
0080	1	Reducer; DN 16/DN 25, aluminum	052 2160

Table 4-29. Springer - Kit for ETD (P/N 124 1530)

Pos. No.	Qty.	Designation	Part No.
0010	1	Plug-in T-piece; 3 x 6mm	112 8140
0020	1	Sleeve 6 mm	104 7320
0030	1	Reducing hose connector, 3.2–>6	123 9220
0040	1	Hose cutter	123 9280
0050	1	Allen wrench 5 mm; long with ball head	123 9290
0060	1	Ring wrench; 10x11, cranked	123 9310
0070	1	Mounting paste; MoS2 - Tube 50 g	124 3890

Table 4-30. Mounting parts - Kit for ETD (P/N 124 1540)

Pos. No.	Qty.	Designation	Part No.
0010	1	T-piece 13 mm	051 2360
0020	2 m	Hose 9 X 3; PVC, black	104 9540
0030	4	Clamping piece 8/16	037 0130
0040	2 m	Hose 13 X 3.5; PVC	069 0720
0050	2	Allen screw, stainless steel; M6; 20 long	045 3420
0060	9	Spring washer; DIN127-B 6-A4	047 0560
0070	1	Cylinder screw; stainless steel, M 4, 12 long	045 0810
0080	2	Spring washer; DIN127-B 4-1.4310	047 0580
0090	1	Nut, stainless steel, M4	046 0220
0100	2	Allen screw, stainless steel; M 6; 25 long	045 3720
0110	3	Allen screw; stainless steel; M6; 45 long	045 3440
0120	2	Nut, stainless steel; M6	046 0520
0130	2	Water draining hose, for ETD	124 4080
0140	0.5 m	Hose; 4 X 1, Teflon	069 0280
0150	1	Clamping ring; stainless steel, NW10/16	114 9200
0160	0.25 m	PEEK capillary; 1/16” x 0.040	124 5940
0170	1	Ferrule, 1/16”, for GVF/16	067 4800
0180	1	Ferrule 1/16" - CTFE, collapsible	122 4700

Electronic Parts of ETD System

Table 4-31. Parts KIT_ETD-ELECTRONICS (P/N 210 8880)

Pos. No.	Qty.	Designation	Part No.
0010	1	INTERCONNEC_ETD-LTQ-ORBITRAP	210 8890
0020	1	Cable Y-ADAPTER/T.PUMP	210 8630
0030	1	Coupling; RJ45 BU/2BU	207 5210

Table 4-31. Parts KIT_ETD-ELECTRONICS (P/N 210 8880), continued

Pos. No.	Qty.	Designation	Part No.
0040	1	Patch cable; 0.51MT RJ45 gray SFTP	208 0870
0050	1	Cable POWER DIS./T-PUMP	208 1200
0060	1	Cable CLT-OFFSET-A	210 8710
0080	1	Cable IOS ETD/ION OPTIC-S	210 8820
0090	1	UNIT_ION OPTIC SUPPLY ETD	210 8920
0100	1	PCB LTQ CABLE DRIVER	209 7780
0110	1	PCB ORBITRAP CABLE RECEIVER	209 7830
0120	1	PCB ETD CABLE RECEIVER	209 7800
0130	1	Cable ETD/LTQ/ORBITRAP-INTERCONNECT 60	210 8940
0140	1	Cable ETD/LTQ/ORBITRAP-INTERCONNECT 36	210 8950
0150	1	Cable ETD/LTQ/ORBITRAP-INTERCON SUPPLY	210 8960
0160	1	Traverse 2, with plate	123 8440
0170	1	Coaxial cable; ETD IOS/ANALOG CTRL, J5554	210 8990
0180	1	Coaxial cable; ETD IOS/ANALOG CTRL, J5555	210 9000
0190	1	Coaxial cable; ETD IOS/ANALOG CTRL, J5556	210 9010
0200	1	Cable ANALOG CTRL / ETD IOS	210 8970
0210	1	Cable ETD IOS/HCD multipole	210 8980
0220	1	Extension cable; 16A C20-C19 2M	209 7050
0230	20	Cable tie; 20 maximum	008 1710
0260	1	ADAPTER_IOS/MULTIPOLE-HCD	210 0410

Parts Lists for the ETD Module

Table 4-32. ETD upgrade from LTQ XL (P/N OPTON-97103)

Pos. No.	Qty.	Designation	Part No.
0010	1	KIT, INTEGRATION, LTQ XL-ETD	98000-62003
0020	1	ASSY, SYSTEM, ETD	98000-60000
0030	1	Kit, Mechanical Pump, ETD*	98000-62005
0040	1	KIT, SHIP, ETD	98000-62004
0050	1	ETD Accessory Kit	98000-62002
0060	1	ETD Reagent Kit*	98000-62008
0070	1	ASSY, TOOL, ION VOLUME INSERTION/REMOVAL	98000-60028
0080	1	Kit, Common Software	97355-62020
0090	1	KIT, SWRE, BIOWORKS 3.3.1 SP1	97355-62005

*Module. see below.df

Table 4-33. Parts Kit, Mechanical Pump, ETD (P/N 98000-0005)

Pos. No.	Designation	Part No.
0010	PUMP, ROTARY VANE, EDWARDS RV3	00108-01-0008
0020	KIT, ACCESSORY, MECHANICAL PUMP, RV3	98000-620007

Table 4-34. Parts Installation Kit Reagent Inlet Module (P/N 98000-62006)

Pos. No.	Qty.	Designation	Part No.
0010	1	TUBING, PEEKsil, 1/16"OD, 100mm LONG, RoHS	00109-02-00020
0020	2	FRLE, 1HOLE, 1/16OD, 0.4mmID, VESP/GRPHT, RO	00101-08-00005
0030	1	FRLE, 2HOLS, 1/16OD, 0.4mmID, VESP/GRPHT, RO	00101-08-00006

Table 4-35. Parts Inlet Valve Seal Kit (P/N 119265-0003)

Pos. No.	Designation	Part No.
0010	Inlet valve seal removal tool	119283-0001
0020	Spool inlet valve seal	119683-0100
0030	O-ring Viton, 0530 ID × 0.082 W	3814-6530

Table 4-36. Parts Filament Assembly DSQ II (P/N 120320-0030)

Pos. No.	Designation	Part No.
0010	Base, filament	119701-20513
0020	Reflector, filament	70001-20517
0030	Filament wire, formed	70001-20516
0040	Shroud, filament	70001-20518
0050	Extraction lens, filament	119701-20520
0060	Box, pastic, 1”×1”×1”, clear/wht	A0301-07532

ETD Reagent Kit

The ETD Reagent Kit (P/N 98000-62008) contains angiotensin I and fluoranthene. See Table 4-37.

Table 4-37. ETD Reagent Kit (P/N 98000-62008)

Pos. No.	Qty.	Designation	Part No.
1	1	Angiotensin I, 1mg	00301-15517
2	1	Fluoranthene, 150mg	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

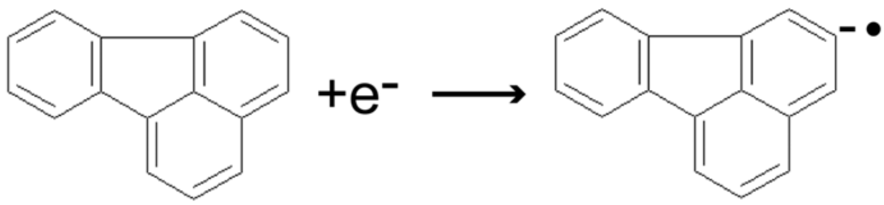
Thermo Fisher Scientific supplies fluoranthene as a two vial kit. One vial contains 150 mg of fluoranthene and the other is the required empty vial.

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 LTQ Orbitrap XL ETD. The fluoranthene radical anion is generated according to the reaction shown in Figure A-1.



Fluoranthene

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).

Note Store and handle all chemicals in accordance with standard safety procedures. The 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. The MSDS also provides 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 way (see the MSDS). ▲

The fluoranthene contained in the ETD Reagent Kit (P/N 98000-62008, see page 4-17) 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.

Glossary

This section lists and defines terms used in this manual. It also includes acronyms, metric prefixes, symbols, and abbreviations.

A ampere

ac alternating current

ADC analog-to-digital converter

AGC™ See Automatic Gain Control™ (AGC).

APCI See atmospheric pressure chemical ionization (APCI).

API See atmospheric pressure ionization (API).

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.

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 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.

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.

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.

b bit

B byte (8 b)

baud rate data transmission speed in events per second

BTU British thermal unit, a unit of energy

°C degrees Celsius

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.

CI See chemical ionization (CI).

CID See collision-induced dissociation (CID).

CLT curved linear trap

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.

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 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.

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

EI electron ionization

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.

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

ESI See electrospray ionization (ESI).

ETD See electron transfer dissociation (ETD).

eV electron volt

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 gram

G Gauss; giga (10^9)

GC gas chromatograph; gas chromatography

GC/MS gas chromatography / mass spectrometer

GUI graphical user interface

h hour

h height

handshake A signal that acknowledges that communication can take place.

HCD Higher Energy Collision Induced Dissociation

header information Data stored in each data file that summarizes the information contained in the file.

H-ESI source 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.

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)

ID inside diameter

IEC International Electrotechnical Commission

IEEE Institute of Electrical and Electronics Engineers

in inch

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.

I/O input/output

ion gauge Measures the pressure in the mass analyzer region (high vacuum region) of the vacuum manifold.

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.

k kilo (10^3, 1000)

K kilo (2^{10}, 1024)

KEGG Kyoto Encyclopedia of Genes and Genomes

kg kilogram

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

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.

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) Ionization by effect of illumination with a beam of laser generated light onto a matrix containing a small proportion of analyte. A mass spectrometric technique that is used for the analysis of large biomolecules.

MB Megabyte (1 048 576 bytes)

MH^+ protonated molecular ion

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.

MSn scan mode The scan power equal to 1 to 10, where the scan power is the power *n* in the expression MSn. MSn 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 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).

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

OT Orbitrap

Ω ohm

p pico (10^{-12})

Pa pascal

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

psig pounds per square inch, gauge

PTM posttranslational modification

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.

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 second

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.

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.

syringe pump A device that delivers a solution from a syringe at a specified rate.

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).

Torr torr

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 Tune Plus (LCQ Series, LXQ, and LTQ) or Tune Master (TSQ Quantum) window and saved as the file type .LCQTune, .LTQTune, or.TSQTune, respectively.

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 atomic mass unit

UHV ultra high vacuum

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 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 filtered air or to the gas supply. A solenoid-operated valve.

vol volume

w width

W watt

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