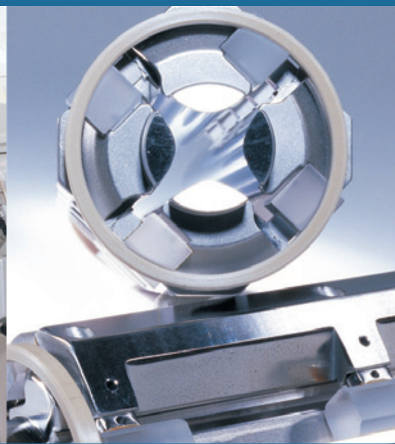
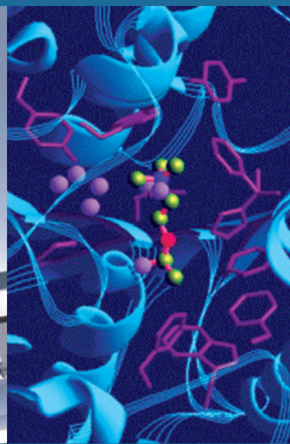
Thermo Fisher Scientific

LTQ Orbitrap Discovery™

Hardware Manual

Revision B - 1225850





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EMV (Störfestigkeit): EMC (immunity) 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)
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(Jörg Behrens)

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San Jose CA, USA, 8/25/2008

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(Bret Johnson)

Read This First

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

About This Guide

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

Who Uses This Guide

This *LTQ Orbitrap Discovery 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 Discovery.
- Chapter 2: "Basic System Operations" provides procedures for shutting down and starting up the LTQ Orbitrap Discovery.
- Chapter 3: "User Maintenance" outlines the maintenance procedures that you should perform on a regular basis to maintain optimum MS detector performance.
- Chapter 4: "Replaceable Parts" lists the replaceable parts for the MS detector and data system.

Related Documentation

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

- *LTQ Orbitrap XL / LTQ Orbitrap Discovery Preinstallation Requirements Guide*
- *LTQ Orbitrap Discovery 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

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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 Discovery 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 Discovery. It contains the following topics:

General Description

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

Figure 1-1. LTQ Orbitrap Discovery front view

Figure 1-2 on page 1-3 shows the schematic view of the LTQ Orbitrap Discovery. The LTQ Orbitrap Discovery consists of three main components, 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 HCD (Higher Energy Collisional Dissociation) experiments is available as option for LTQ Orbitrap Discovery. The feature will be not available if the instrument is not equipped with this option.

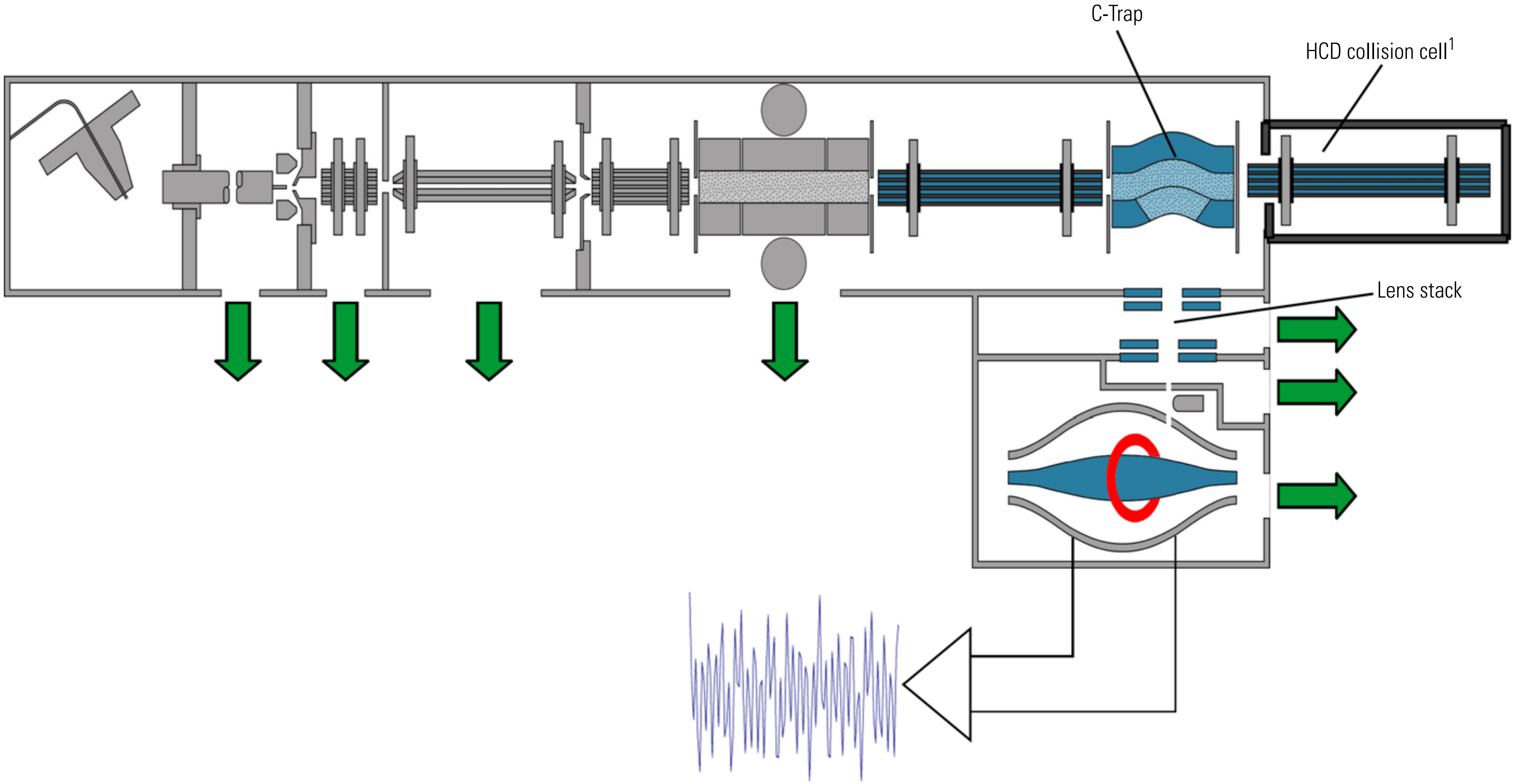

Figure 1-2. Schematic view of the LTQ Orbitrap Discovery

[1]HCD is an option for LTQ Orbitrap Discovery. The feature will be not available if the instrument is not equipped with this option.

Wheels at the bottom side of the instrument facilitate positioning the LTQ Orbitrap Discovery at the intended place in the laboratory. The instrument is designed to be placed with its rear panel against a wall. To ensure a sufficient air flow for cooling the instrument, spacers on the rear panel provide for minimum distance to the wall.

The mains inlet as well as a power outlet for peripheral devices (data system, for example) are located at the right side of the instrument. Rotary pumps are hidden under the linear trap and accessible from the front. The left side panel and the front panel are mounted on hinges and the right side panel is removable.

The top lid opens upwards to allow easy access for Field Engineers from the top. See Figure 1-3.

Figure 1-3. Top lid 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 Discovery has the following measuring properties:

Resolution (apodized)	30000 (FWHM) @ m/z 400 with a detect time of 400 ms Minimum resolution 7500, maximum resolution 30000 @ m/z 400
Mass Range	m/z 50–2000; m/z 200–4000
Mass Accuracy	<5 ppm RMS for 8 h period with external calibration, <2 ppm RMS with internal calibration
Dynamic Range	>10000 between mass spectra, >4000 between highest and lowest detectable mass in one spectrum
MS/MS	MS/MS and MS^n scan functions

Control Elements

The LTQ Orbitrap Discovery 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.) While the Power LED is directly controlled by the 3 × 230 V input, all other LEDs are controlled by the power distribution board (Refer to topic "Power Distribution Board" on page 1-39). Table 1-1 explains the function of the various LEDs.

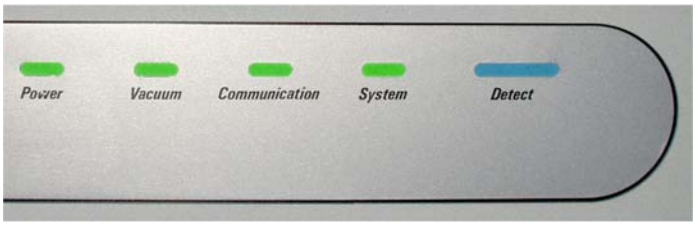

Figure 1-4. System status LEDs

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 Product Short Name

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	Instrument is scanning
	Off	Instrument 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 Discovery. Located here are the control panels, switches, and the ports for the external connections (mains supply, gases, Ethernet communication, and cooling water).

Figure 1-5. Right side of the LTQ Orbitrap Discovery

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.

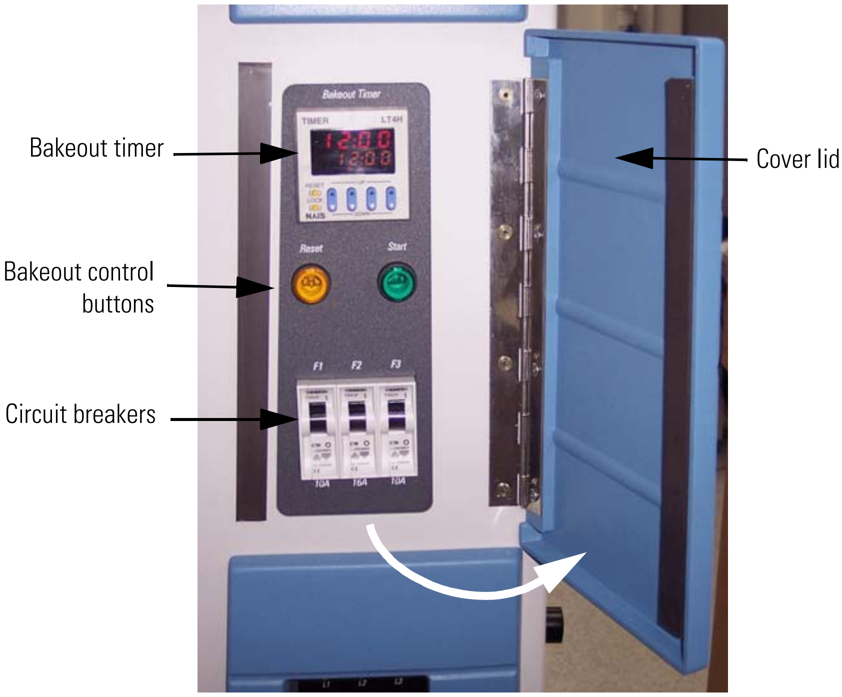

Figure 1-6. Upper control panel

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 Discovery 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 Discovery

Circuit breaker	Ampere	LED	Instrument parts
F1	10	L1	Power Distribution
F2	16	L2	Linear ion trap
F3	10	L3	Multiple socket outlets (Data system, 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 Discovery 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.)

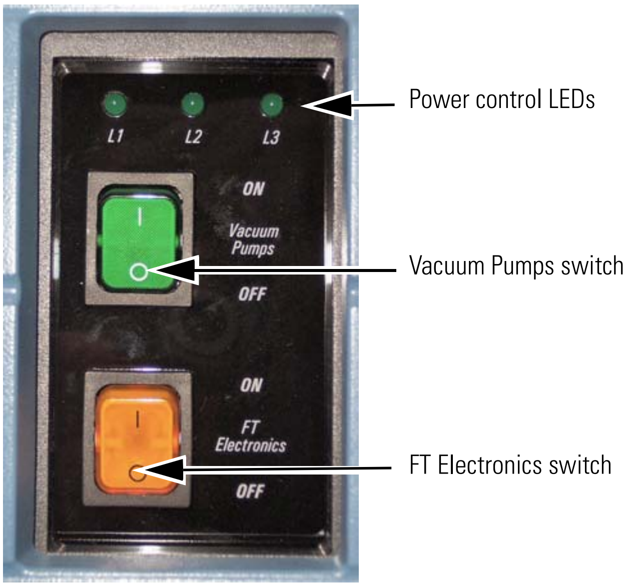

Figure 1-7. Power control panel with power control LEDs and switches

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 1-39)
- Pumps (Refer to the topic "Vacuum System" on page 1-19)
- Temperature controller (Refer to the topic "Temperature Controller Board" on page 1-48)
- 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 Discovery (and linear ion trap as well, including the vacuum pumps).

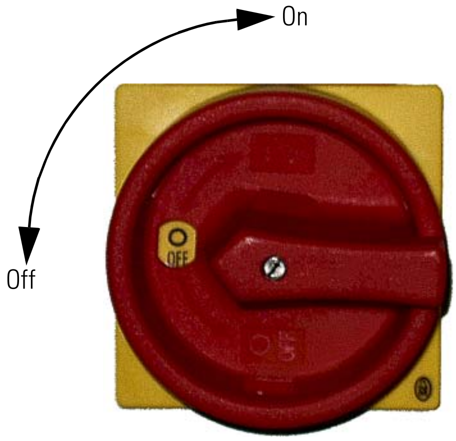

Figure 1-8. Main power switch

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 1-28.) A Teflon® hose connects the instrument to the nitrogen gas supply. An analogous port is used for the HCD collision gas supply.[1] Metal tubing connects the instrument with the helium gas supply. (See also topic "Gas Supply" on page 1-25.) Located at the top are two ports for Ethernet cables for connecting the LTQ Orbitrap Discovery 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.

[1]HCD is an option for LTQ Orbitrap Discovery. The feature will be not available if the instrument is not equipped with this option.

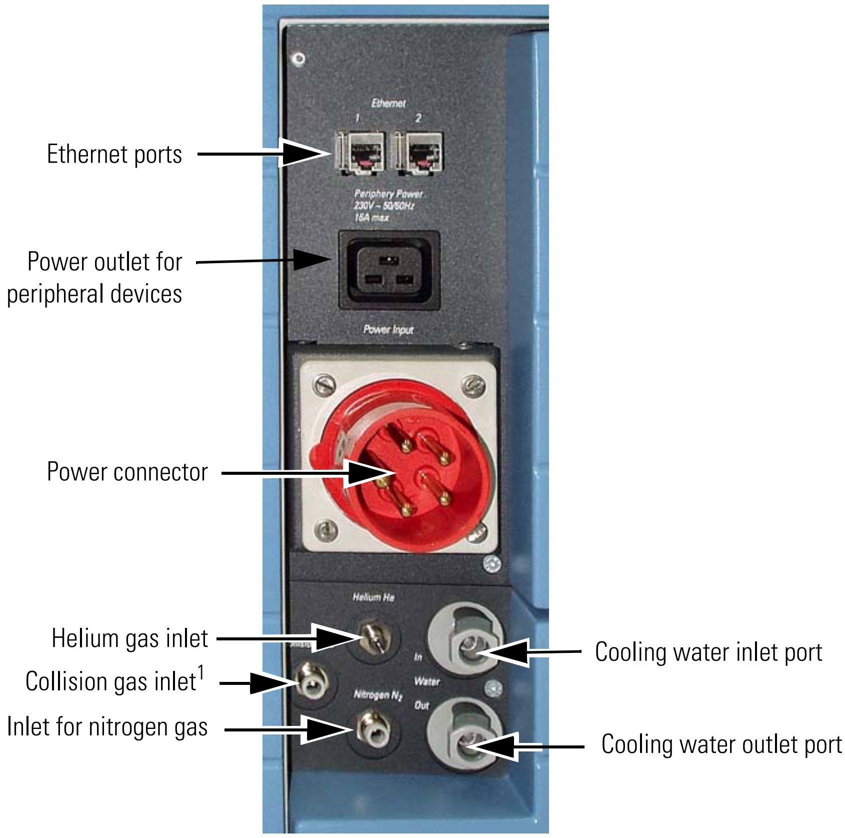

Figure 1-9. External connections to the LTQ Orbitrap Discovery

The power outlet for peripheral devices (data system, for example) is located above the mains supply port. The outlet provides the mains supply for the peripherals via a multiple socket outlet.

Caution **Do not connect the recirculating chiller to the peripherals power outlet!**
Furthermore, make sure that the maximum current drawn from the power outlet does not exceed 16 A. Overloading it (by connecting to many pieces of equipment to the multiple socket outlet, for example) may destroy the outlet by excessive heating. ▲

[1]Not used in the standard version of the LTQ Orbitrap Discovery.

Linear Ion Trap

The LTQ Orbitrap Discovery 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 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 1-18 on page 1-21. The Product Short Name provides power for the linear ion trap – and for the data system.

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 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.

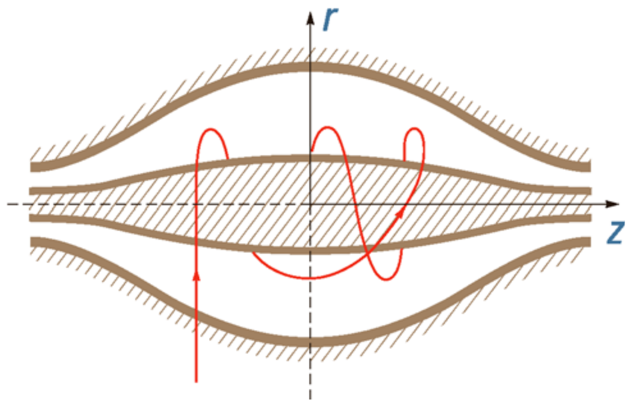

Figure 1-10. Schematic view of the Orbitrap cell and example of a stable ion trajectory

Measuring Principle

In the mass analyzer shown in Figure 1-10, stable ion 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 ion mass-to-charge ratio *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 octapole (Oct 1) 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 1-50.) Trap and gate DC voltages as well as RF voltages to octapole 1 are all provided by the ion optic supply board. (See page 1-46.) High voltages to the lenses are provided by the high voltage power supply board. (See page 1-53.)

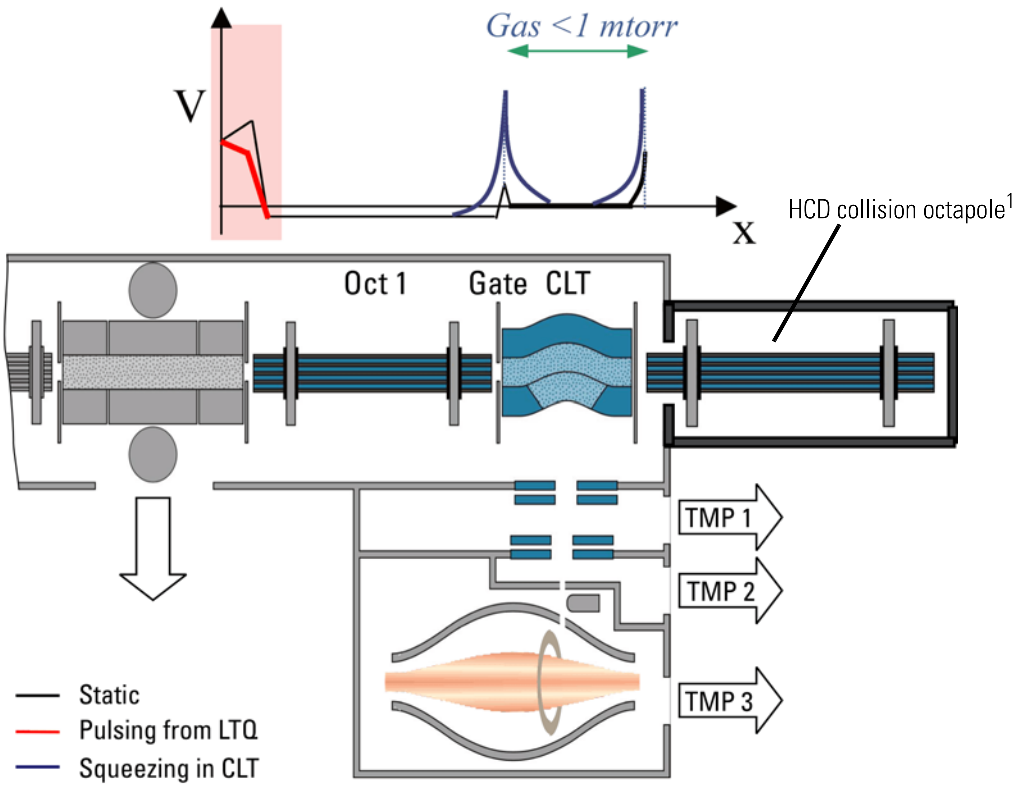

Figure 1-11. Layout of the instrument, also showing the applied voltages

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 curved trap and the subsequent lenses, the ion beam converges on the entrance into the Orbitrap. The lenses form also differential pumping slots and cause

[1]HCD is an option for LTQ Orbitrap Discovery. The feature will be not available if the instrument is not equipped with this option.

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/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.

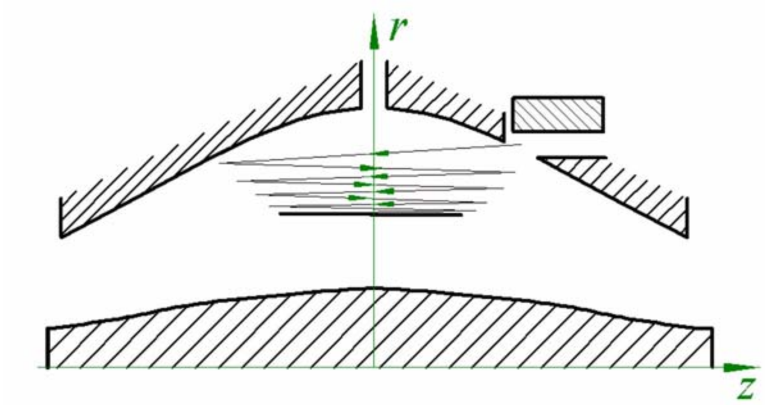

Figure 1-12. Principle of electrodynamic squeezing of ions in the Orbitrap as the field strength is increased

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.

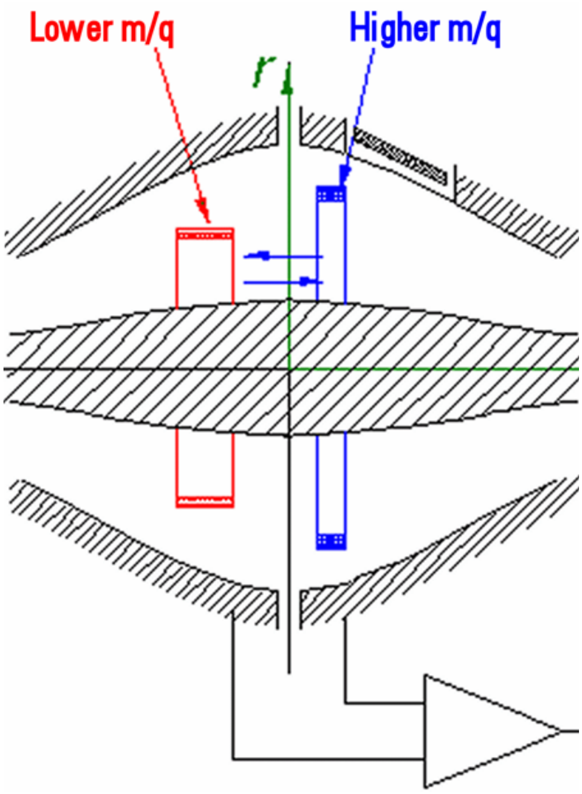

Figure 1-13. Approximate shape of ion packets of different m/q after stabilization of voltages

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, while 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 1-48.

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 1-32 on page 1-45.

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 Discovery. See topic "Cooling Water Circuit" on page 1-28 for further information.

HCD Collision Cell

HCD is an option for LTQ Orbitrap Discovery. The feature will be not available if the instrument is not equipped with this option.

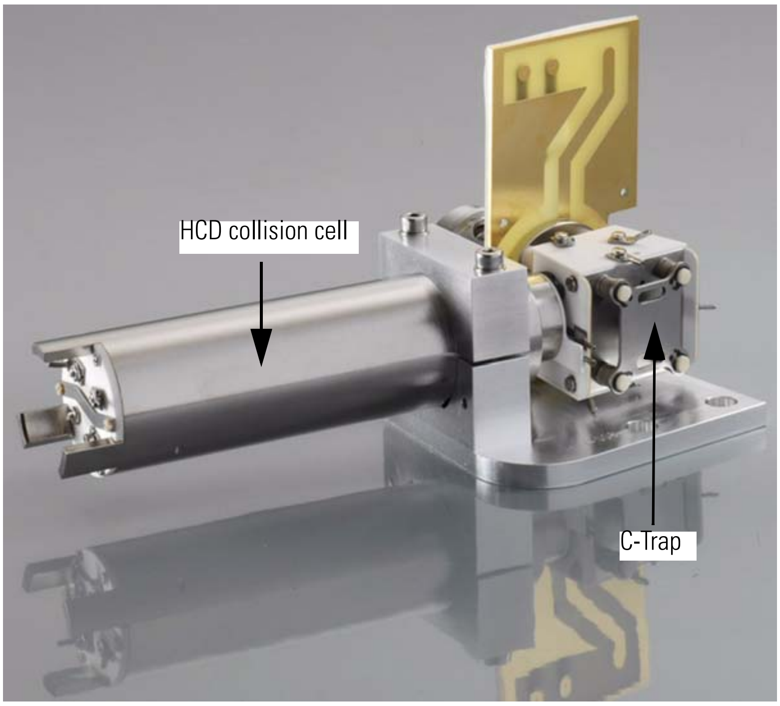

Figure 1-14. HCD collision cell and C-Trap

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. Figure 1-14 on page 1-18 shows a close-up view of the configuration.

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 1-25 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 1-46.)

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 Discovery Getting Started* manual for more information.

Vacuum System

Figure 1-15 shows a schematic overview of the vacuum system. The Orbitrap 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)

The forepumps of the linear trap provide the forevacuum for the turbopumps.

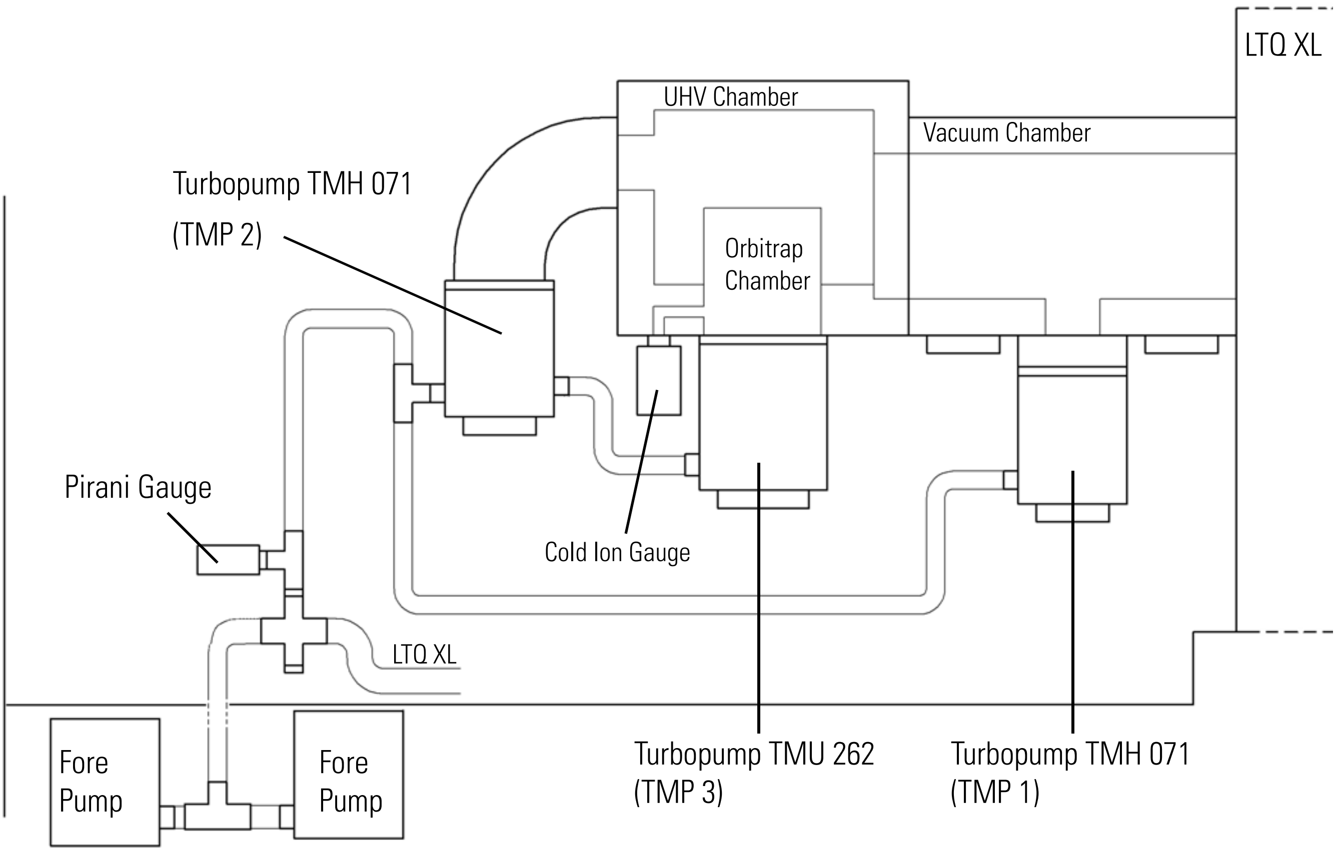

Figure 1-15. Schematical view of vacuum system (C-Trap compartment not shown)*

*For an abridged version of the parts list, see Table 4-7 on page 4-3.

Turbopumps

All parts of the system except for the Orbitrap analyzer are mounted in a aluminum vacuum chamber evacuated by a 60 L/s turbopump (**TMP 1**, see Figure 1-16). 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.

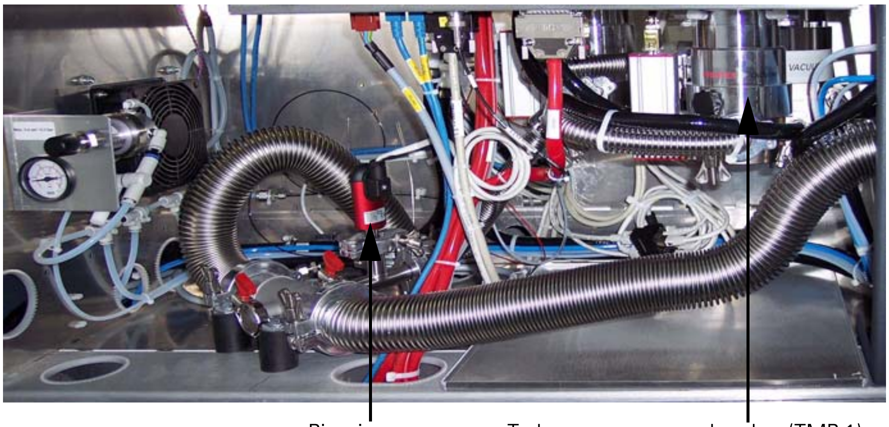

Figure 1-16. Vacuum components on the left instrument side

The UHV chamber is evacuated down to 10^{-8} mbar pressure range by a 60 L/s UHV turbopump (**TMP 2**, see Figure 1-17).

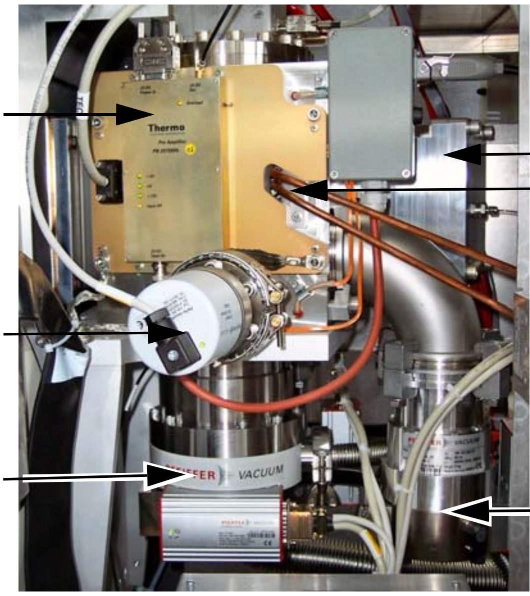

Figure 1-17. Vacuum components on the right instrument side

[1]HCD is an option for LTQ Orbitrap Discovery. The feature will be not available if the instrument is not equipped with this option.

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 1-17 on page 1-20). All turbopumps are equipped with TC 100 control units (manufacturer: Pfeiffer).

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*.

Forevacuum Pumps

The rotary vane pumps from the linear trap serve as forepumps for the two smaller turbopumps (TMP 1 and TMP 2). 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 1-18.

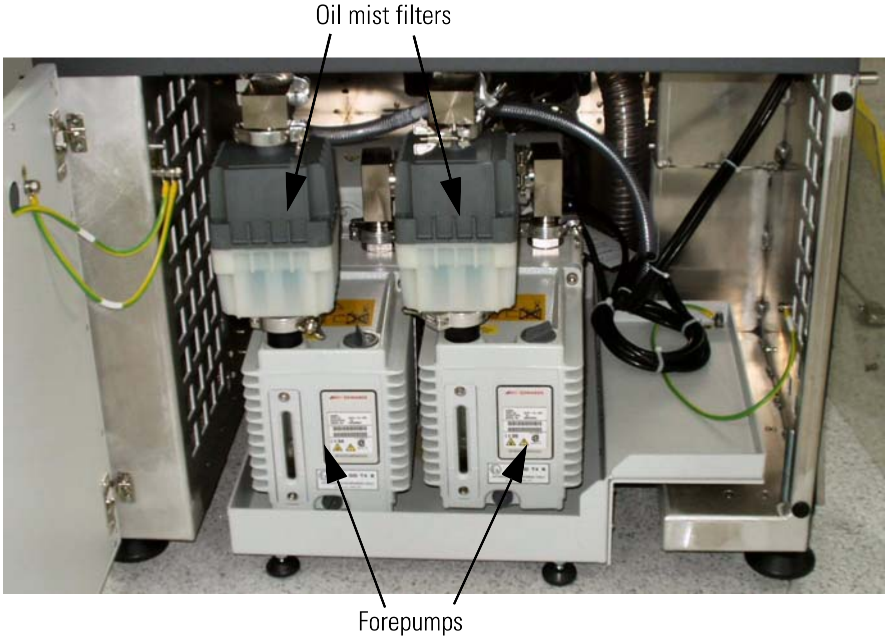

Figure 1-18. Forepumps cabinet

To minimize the ingress of pump oil into the exhaust system, the outlets of the forepumps are fitted to oil mist filters. See page 3-6 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 on/off 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.

Vacuum System Controls

The power distribution board controls all turbopumps via voltage levels. Refer to topic "Power Distribution Board" on page 1-39. 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 1-37.) The linear ion trap has a separate turbopump controller.

Vacuum Gauges

The vacuum is monitored by several vacuum gauges:

- The forevacuum of the LTQ Orbitrap Discovery is monitored by an Active Pirani gauge (TPR 280, manufacturer: Pfeiffer) connected to the LTQ Orbitrap Discovery forevacuum line. See photo right and Figure 1-16 on page 1-20.

- The high vacuum of the LTQ Orbitrap Discovery is monitored by a Cold Ion Gauge (IKR 270, manufacturer: Pfeiffer) connected to the UHV chamber. See Figure 1-17 on page 1-20. Since the gauge would be contaminated at higher pressures, it is only turned on 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.

The vacuum gauges of the LTQ Orbitrap Discovery are connected to the power distribution board that directly responds to the pressure values. (Refer to the topic "Power Distribution Board" on page 1-39.) The analog values are digitized by the instrument control board. (Refer to the topic "Instrument Control Board" on page 1-37.) They are then sent as readout values to the data system.

Switching on the Vacuum System

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

1. After the Vacuum Pumps switch is switched On, the pumps of the linear ion trap and the LTQ Orbitrap Discovery are run up. The Pirani gauge (see above) controls the LTQ Orbitrap Discovery 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 Discovery 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 1-39.) 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 1-27.)

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

Figure 1-19 shows a schematical view of the gas supply in the instrument. The LTQ Orbitrap Discovery uses at least two gases for operation:

- Nitrogen,
- Helium, and
- Argon (optional as HCD collision gas)[1].

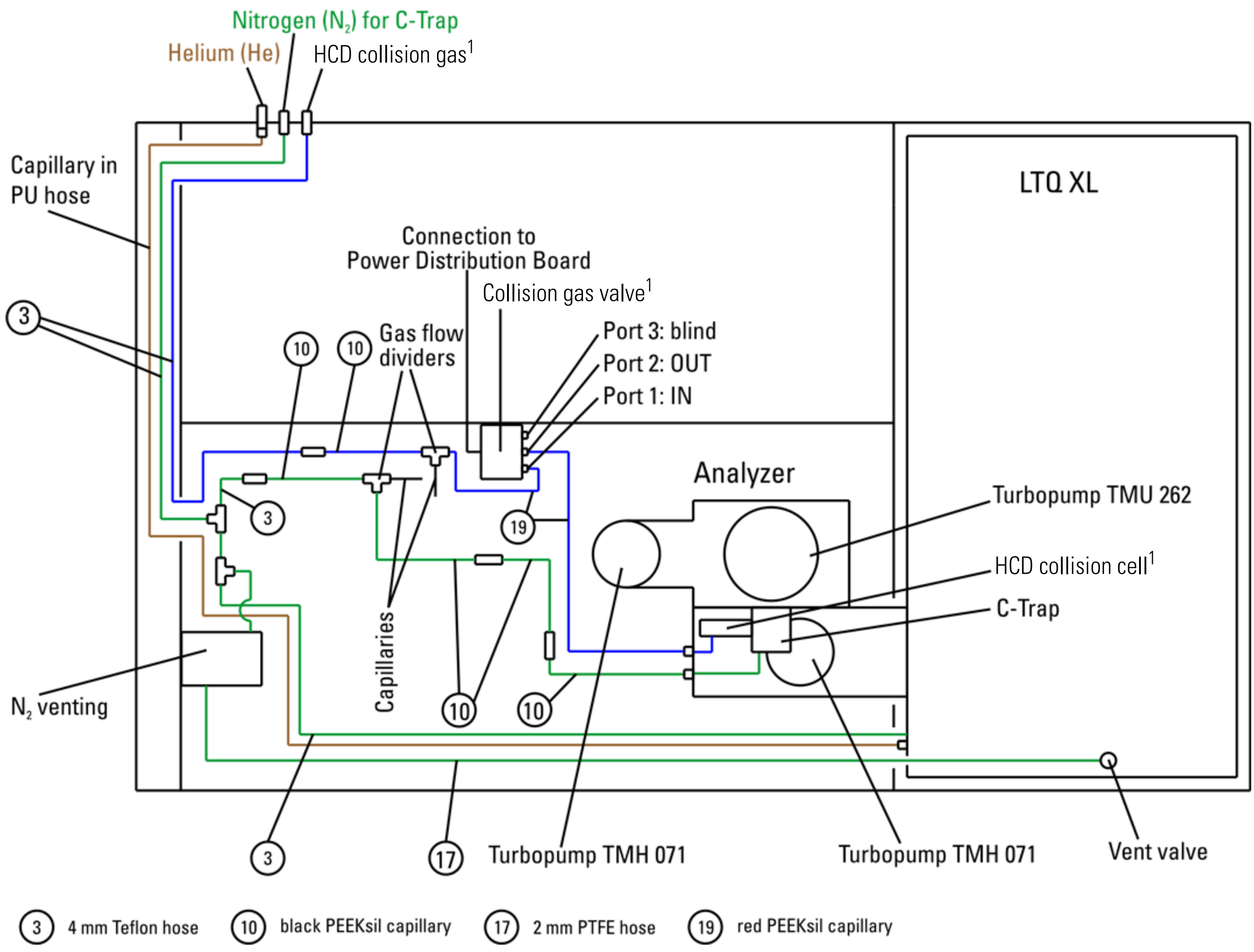

Figure 1-19. Schematical view of the gas supply*

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

[1]HCD is an option for LTQ Orbitrap Discovery. The feature will be not available if the instrument is not equipped with this option.

The linear trap requires high-purity (99%) nitrogen for the API sheath gas and auxiliary/sweep gas. The Orbitrap uses nitrogen as collision gas (bath gas) for the curved linear trap. The linear trap requires ultra-high purity (99.999%) helium for the collision gas.
Nitrogen is also used as collision gas for the optional HCD octapole. If 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. Nitrogen gas and HCD collision gas are both led via Teflon tubing to the right side of the LTQ Orbitrap Discovery.

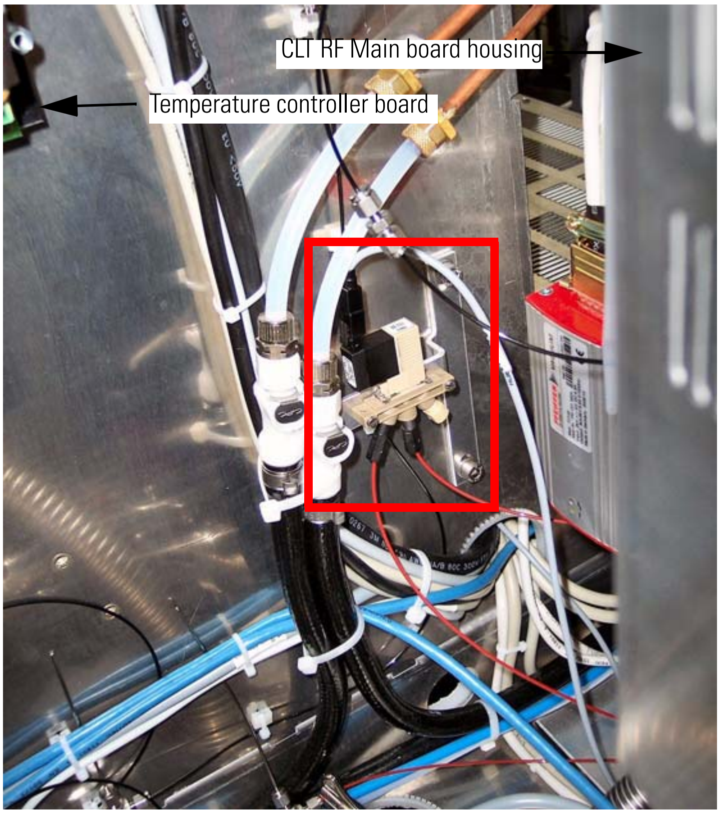

Figure 1-20. Valve for HCD collision gas

Part of the 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 gas pressure to the C-Trap is kept constant by using an "open-split" interface (gas flow divider, see Figure 1-21 on page 1-27). 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 in PEEK tubing).

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.

The instrument is vented with nitrogen from the same tubing that supplies the LTQ XL sheath gas. See Figure 1-19 above. 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 Discovery. See Figure 1-21.

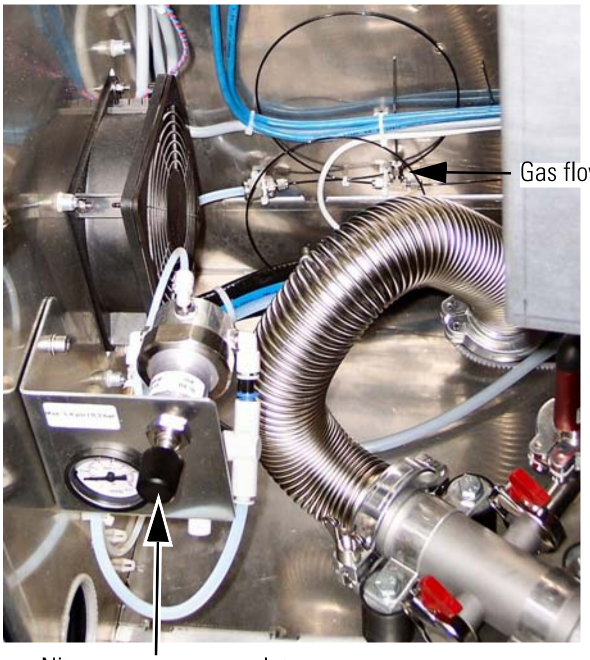

Figure 1-21. Nitrogen pressure regulator and gas flow divider

Cooling Water Circuit

Figure 1-22 on page 1-28 shows a schematical view of the cooling water circuit in the LTQ Orbitrap Discovery. 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 2. Then it passes through the heating element (Peltier element) that keeps constant (±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.

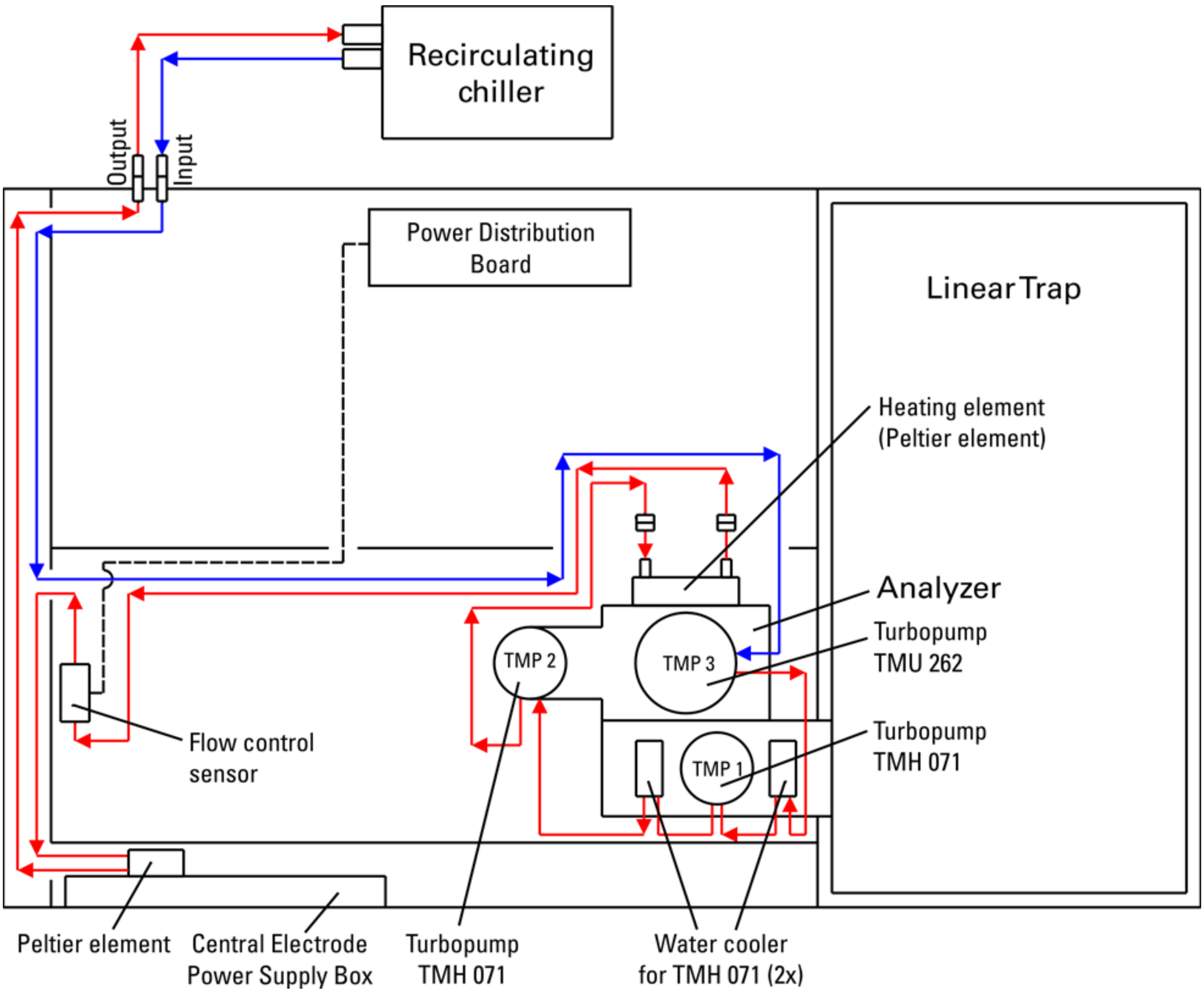

Figure 1-22. Schematical view of cooling water circuit*

*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 Discovery 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 3-7. 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 Discovery 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 various electronic boards of the LTQ Orbitrap Discovery. For each board, its respective location and function are given. If applicable, the diagnostic LEDs on the board are described.

The electronics of the LTQ Orbitrap Discovery 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 Discovery diagnostics, which is accessible from the Tune Plus window. ▲

Linear Ion Trap Electronics

The linear ion trap is connected to the LTQ Orbitrap Discovery main power switch. The linear ion trap has a sheet metal back cover. Figure 1-23 shows the electronic connections at the rear side of the linear trap.

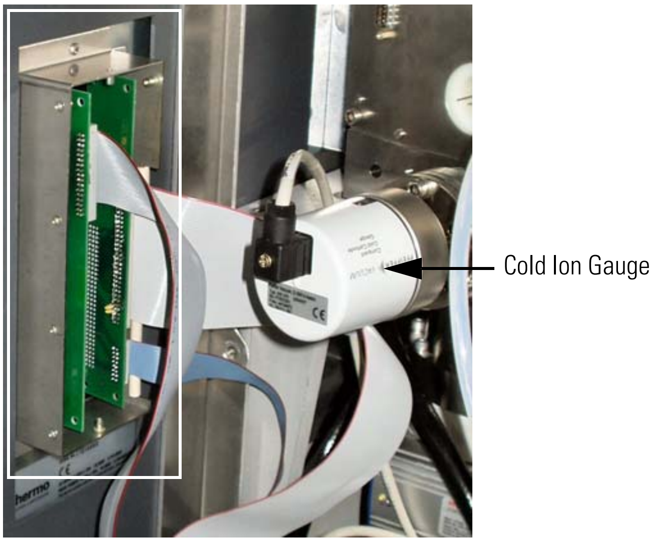

Figure 1-23. Electronic connections to linear trap (covers removed)

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

- Data communication with the internal computer of the LTQ Orbitrap Discovery. Refer to the topic "Electronic Boards at the Right Side of the Instrument" on page 1-32.

- Signal communication (SPI bus) with supply information for the instrument control board. Refer to the topic "Instrument Control Board" on page 1-37.

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 1-24 shows the parts of the instrument when the right side panel is opened. A transparent cover protects the lower part.

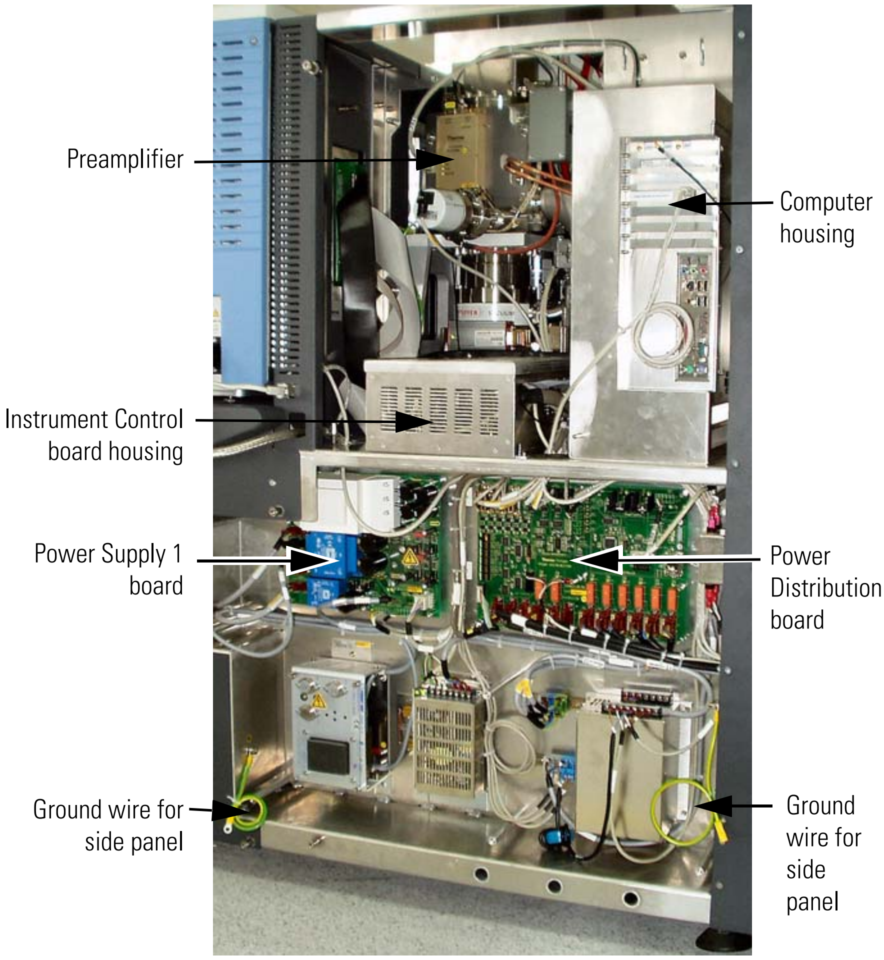

Figure 1-24. Electronic boards on the right side of the instrument

The side panel is connected to the instrument frame by two green/yellow ground wires. See bottom of Figure 1-24. 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!

Preamplifier

Figure 1-25 shows the preamplifier (P/N 207 8900)[1]. The preamplifier is located in a housing next to the Cold Ion Gauge.

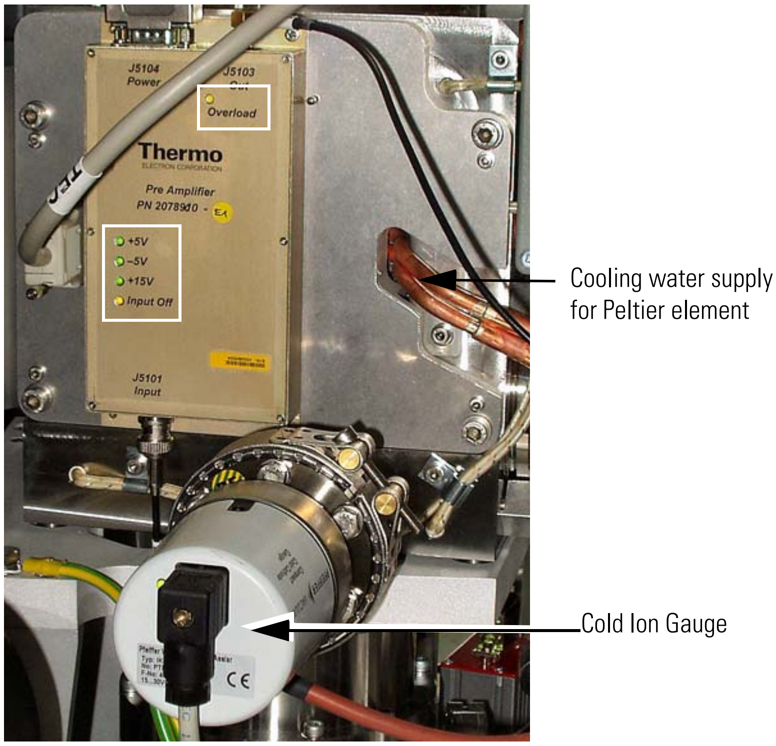

Figure 1-25. Preamplifier board

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 1-3 on page 1-34. The positions of the diagnostic LEDs on the board are indicated by white rectangles in Figure 1-25.

[1] Part number of complete unit.

Table 1-3. 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 1-26 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.

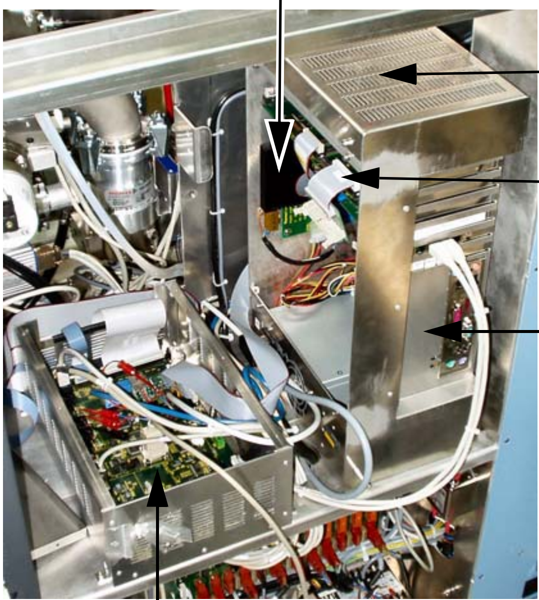

Figure 1-26. Data Acquisition unit (covers removed)

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 1-27 shows the data acquisition digital PCI board (P/N 206 0501). It is an add-on board to the internal computer (See Figure 1-26 on page 1-34.).

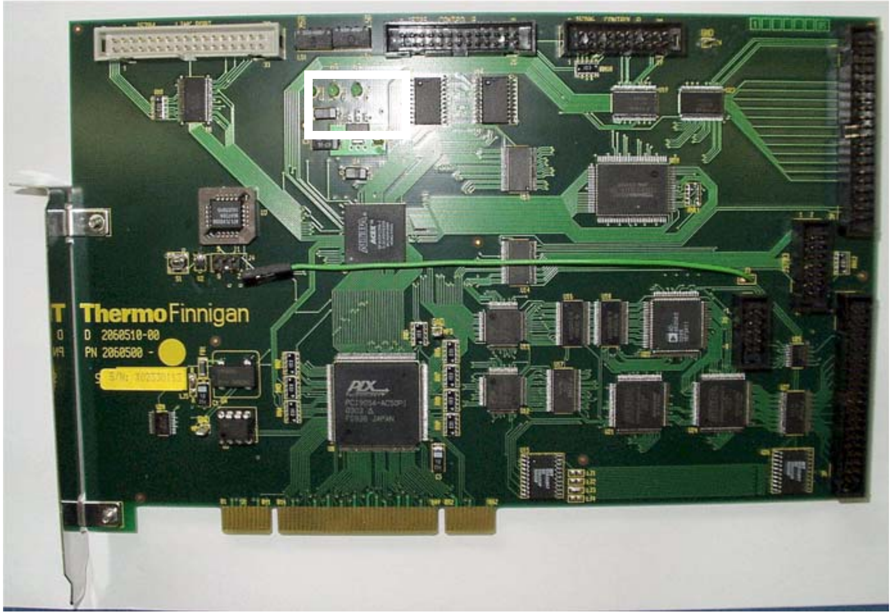

Figure 1-27. Data Acquisition Digital PCI board

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.

While precision timing is derived from the data acquisition analog board, 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 Discovery 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 1-4 on page 1-36 show the status of the board. The position of the LEDs on the board is indicated by a white rectangle in Figure 1-27.

Table 1-4. 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 1-28 shows the data acquisition analog board (P/N 206 4150).

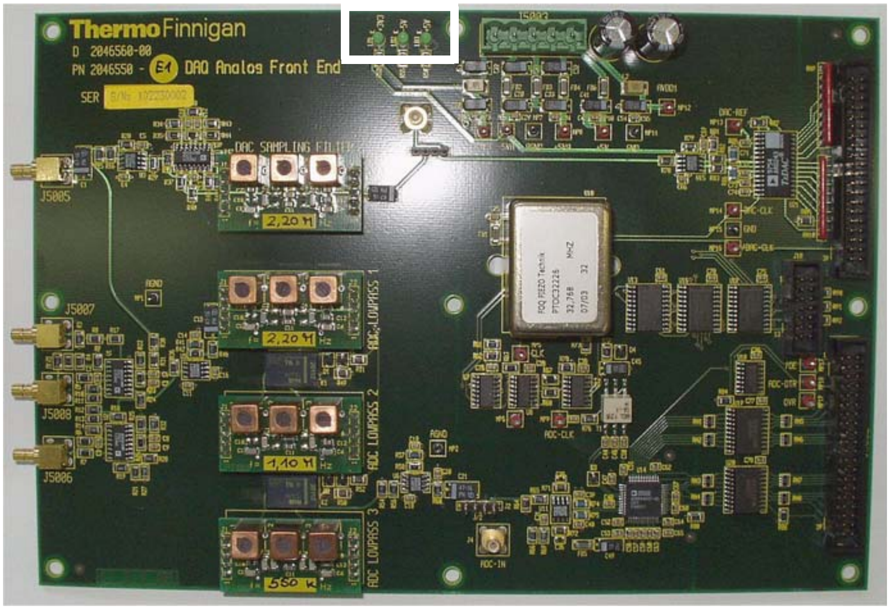

Figure 1-28. Data Acquisition Analog board

This board is an add-on board to the mainboard of the internal computer. See Figure 1-26 on page 1-34. 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 1-5 on page 1-37 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 1-28.

Table 1-5. 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 1-26 on page 1-34.

The diagnostic LEDs listed in Table 1-6 show the status of the voltages applied to the board.

Table 1-6. 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 1-29 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 Discovery 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 1-39.) Turbopumps (Refer to the topic "Vacuum System" on page 1-19.) are attached to a serial port connector and this is connected via the signal lines to the linear ion trap.

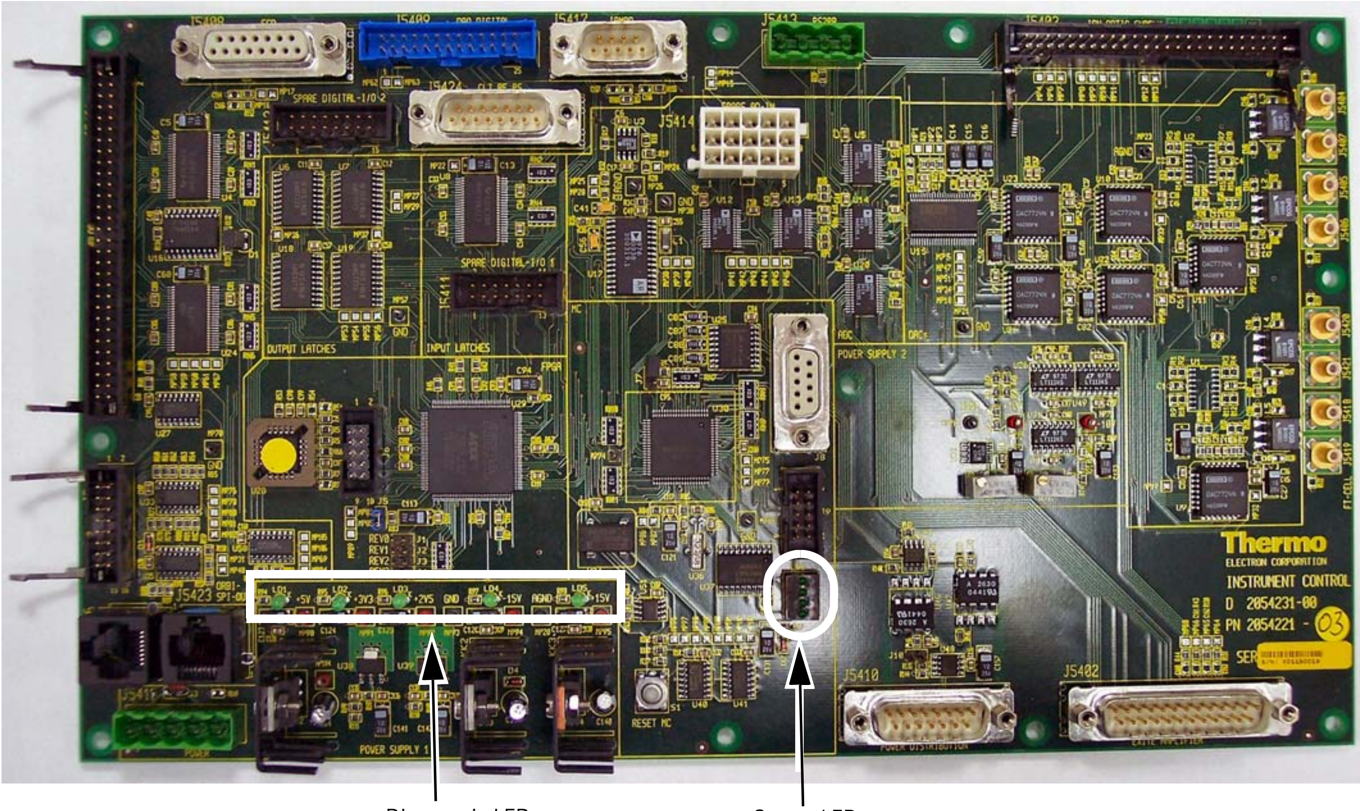

Figure 1-29. Instrument Control board

The diagnostic LEDs listed in Table 1-7 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 1-29.

Table 1-7. 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 1-8 on page 1-39. The position of the status LEDs on the board is indicated by a white oval in Figure 1-29 on page 1-38.

Table 1-8. 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 1-30 shows the power distribution board (P/N 210 1320)[1]. It is located at the bottom of the right side of the instrument.

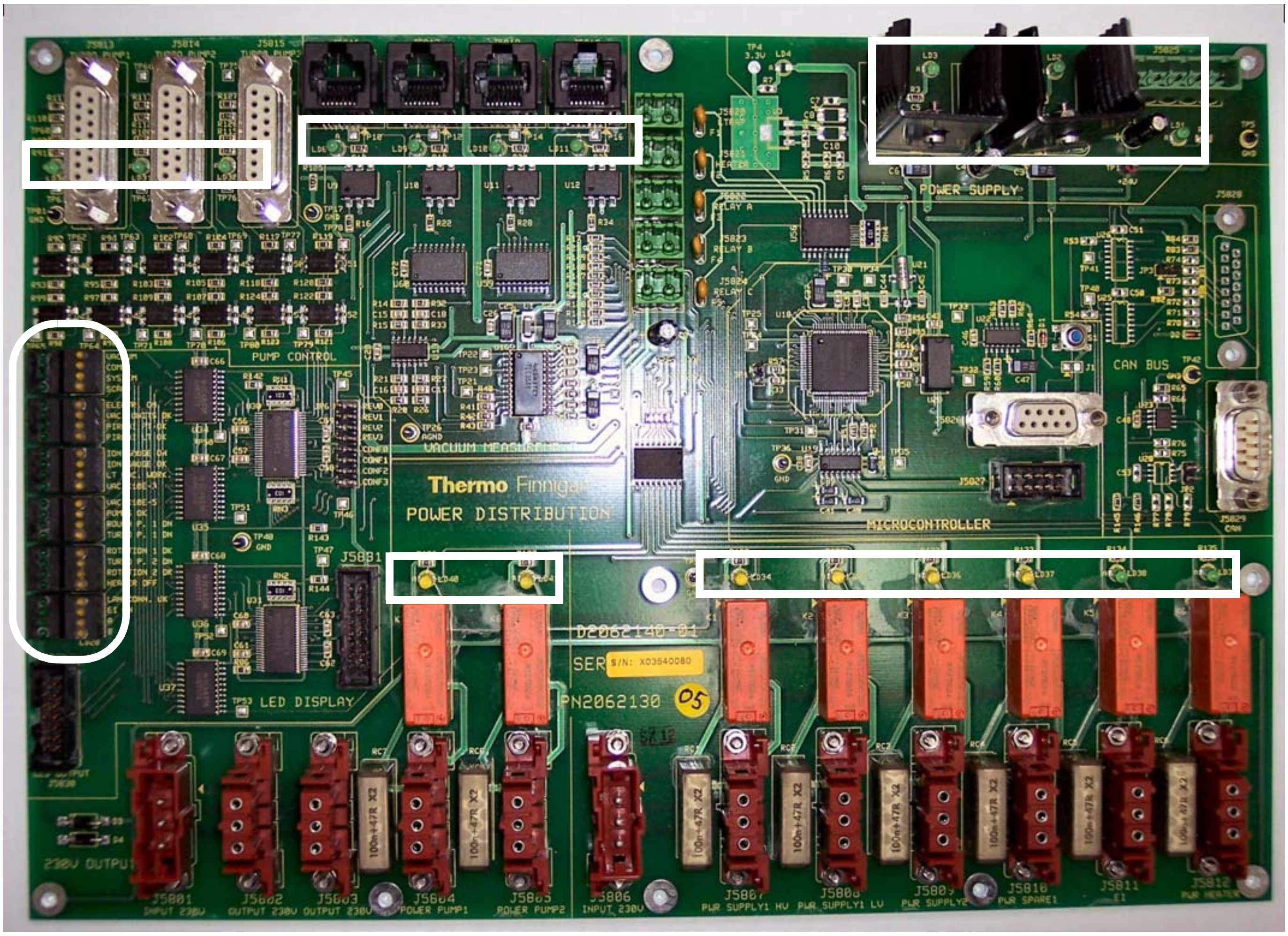

Figure 1-30. Power Distribution board

[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 1-9 on page 1-41) 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 1-30 on page 1-39.

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 1-37.)

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 1-30 on page 1-39.

Table 1-9. 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 Discovery off	Forevacuum > 10^{-2} mbar
Ion Gauge OK	Penning LTQ Orbitrap Discovery 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.

Depending on user actions, the power distribution is switched to various working modes by the hardware. See Table 1-10.

Table 1-10. Working modes of the Power Distribution board

	Action	Consequences
a.	Main switch off	Complete system including linear ion trap and multiple socket outlets (data system, 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 1-11 shows the possible operating states of the power distribution.

Table 1-11. 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 Discovery forevacuum pump: 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 1-11. 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 Discovery $>10^{-1}$ mbar • Penning gauge LTQ Orbitrap Discovery $>10^{-3}$ 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 Discovery without data link, keeps on running
10.	FT Electronics switch LTQ Orbitrap Discovery off	LTQ Orbitrap Discovery electronics switched off, pumps keep on running; LTQ Orbitrap Discovery without data link, keeps on running
11.	Failure of linear ion trap or LTQ Orbitrap Discovery (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 1-31 on page 1-44 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 1-46.) and the instrument control board. (Refer to topic “Instrument Control Board” on page 1-37.)

Figure 1-31. Power Supply 1 board

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

The diagnostic LEDs listed in Table 1-12 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 1-31.

Table 1-12. 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 1-32 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.

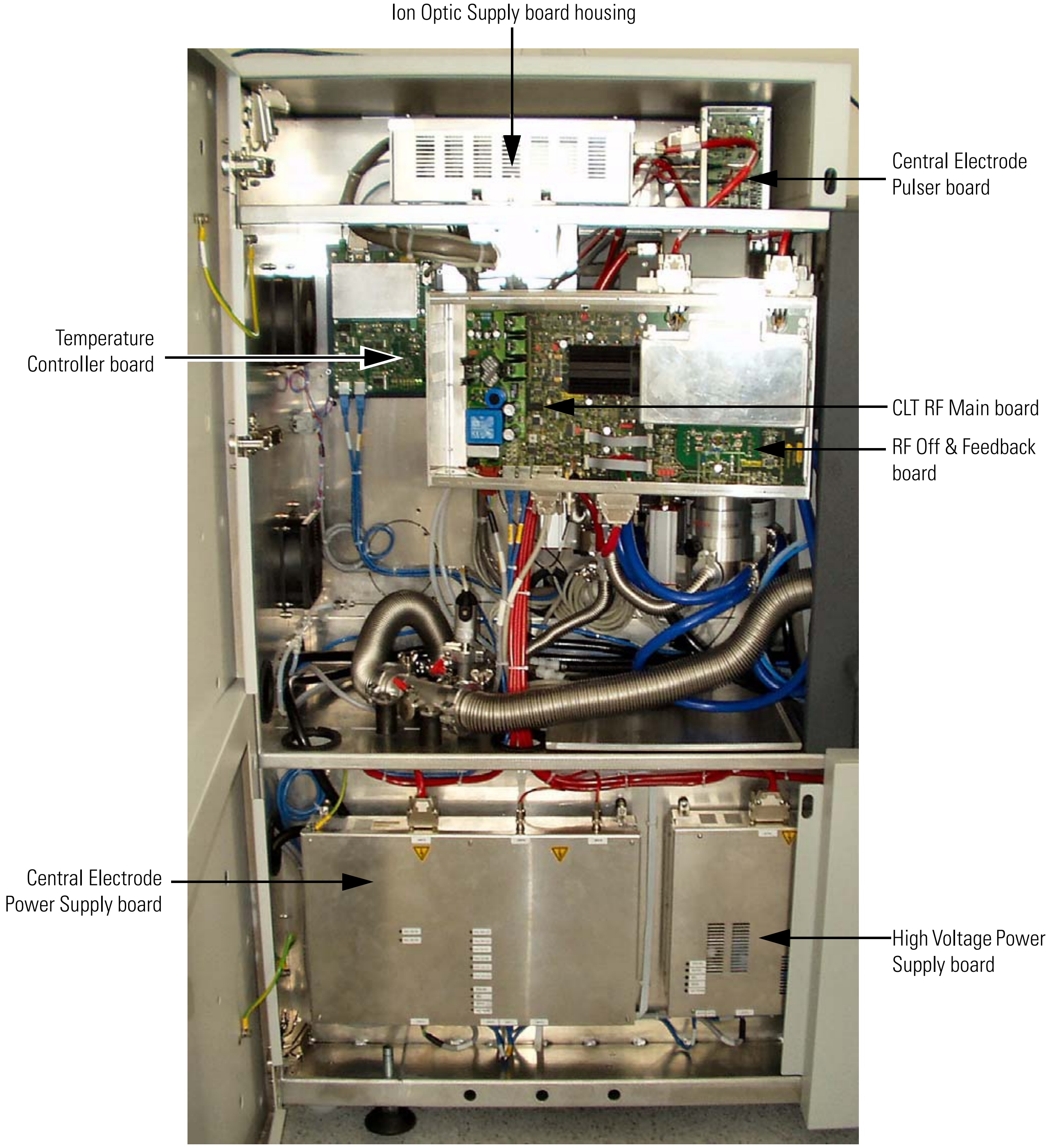

Figure 1-32. Electronic boards on the left side of the instrument

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

Ion Optic Supply Board

Figure 1-33 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 Discovery. It has an RF detector for the RF output control. The board also provides the trap voltage, gate voltage, and reflector dc voltages as well as the RF voltages to the octapole 1 of the Orbitrap. See topic "Orbitrap Analyzer" on page 1-13 for further information. Furthermore, the board provides the voltages for the HCD collision cell.[2] See page 1-18.

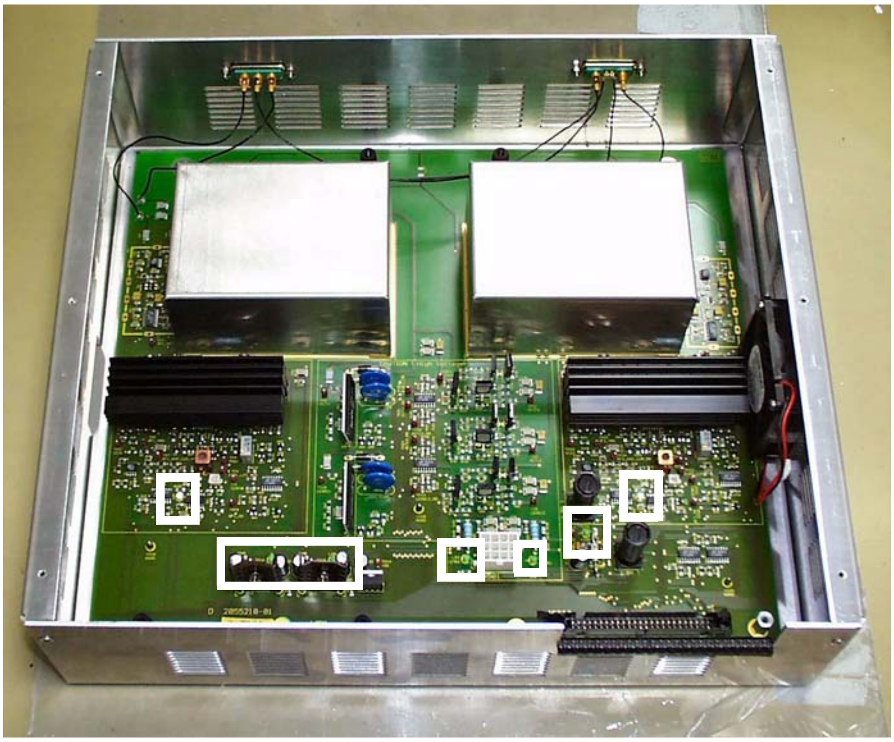

Figure 1-33. Ion Optic Supply board

The diagnostic LEDs listed in Table 1-13 on page 1-47 show the status of applied voltages to the board. The position of the LEDs on the board is indicated by white rectangles in Figure 1-33.

Warning Parts of the board are at high voltage. ▲

[1]Part number of complete unit.

[2]HCD is an option for LTQ Orbitrap Discovery. The feature will be not available if the instrument is not equipped with this option.

Table 1-13. 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.

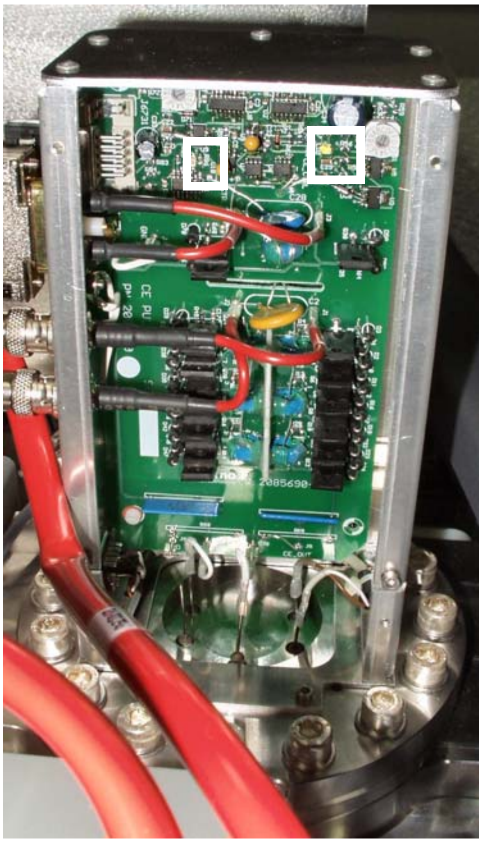

Figure 1-34. Central Electrode Pulser board

[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 1-14 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 1-34 on page 1-47.

Table 1-14. 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 1-32 on page 1-45. 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.

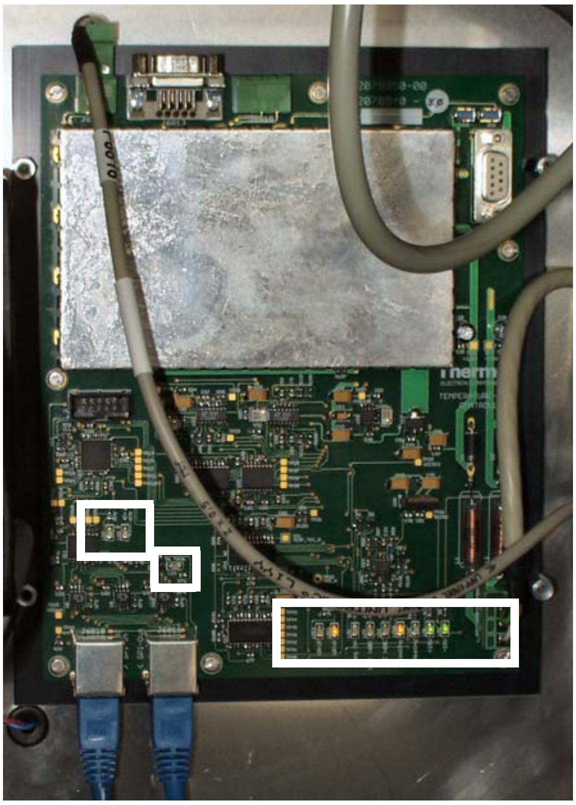

Figure 1-35. Temperature Controller board

The diagnostic LEDs listed in Table 1-15 on page 1-50 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 1-35.

Table 1-15. 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 (C-Trap) 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 1-32 on page 1-45. This board provides an RF voltage ("Main RF") for the curved linear trap (C-Trap). It allows switching off the RF and simultaneous pulsing of each C-Trap electrode. See topic "Orbitrap Analyzer" on page 1-13 for further information. The board communicates with the instrument control board via an SPI bus.

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 1-36 on page 1-51.

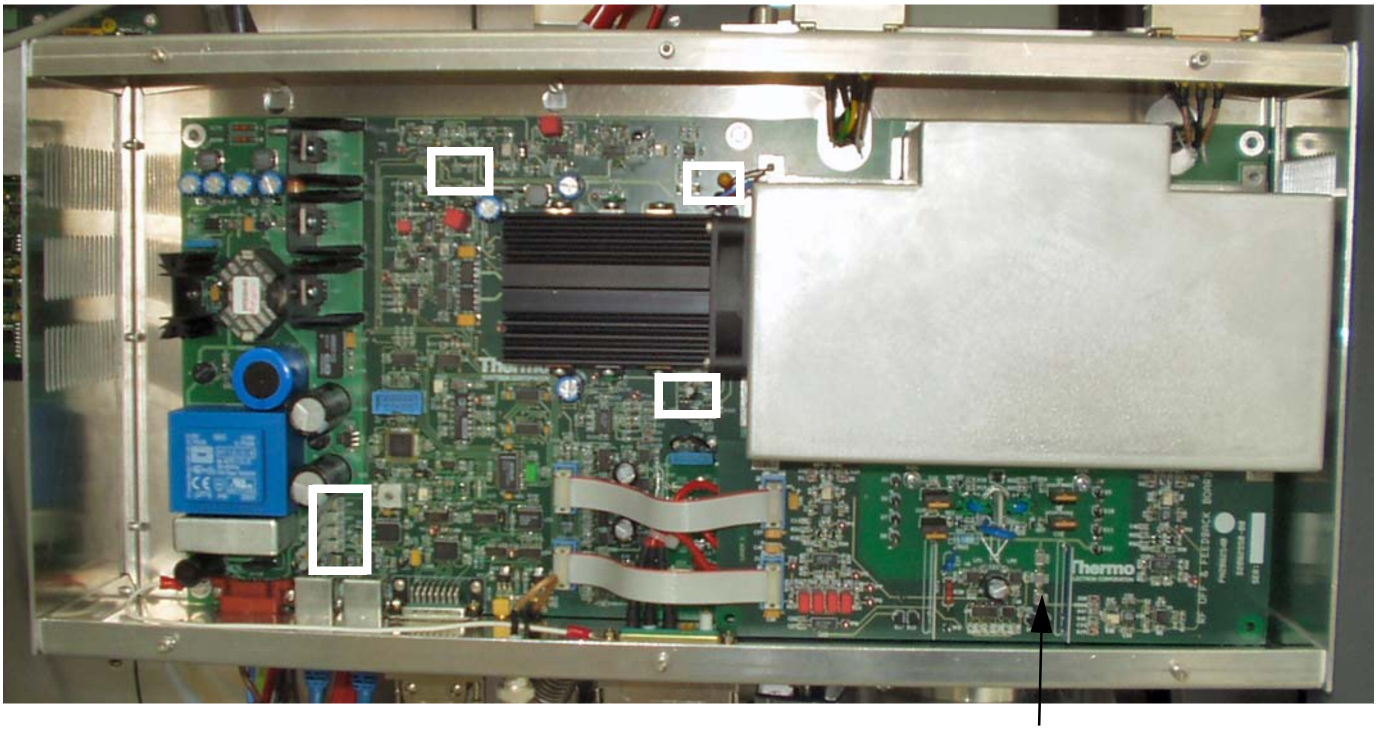

Figure 1-36. CLT RF unit (cover removed)

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 1-36.

Table 1-16. 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

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 1-37.

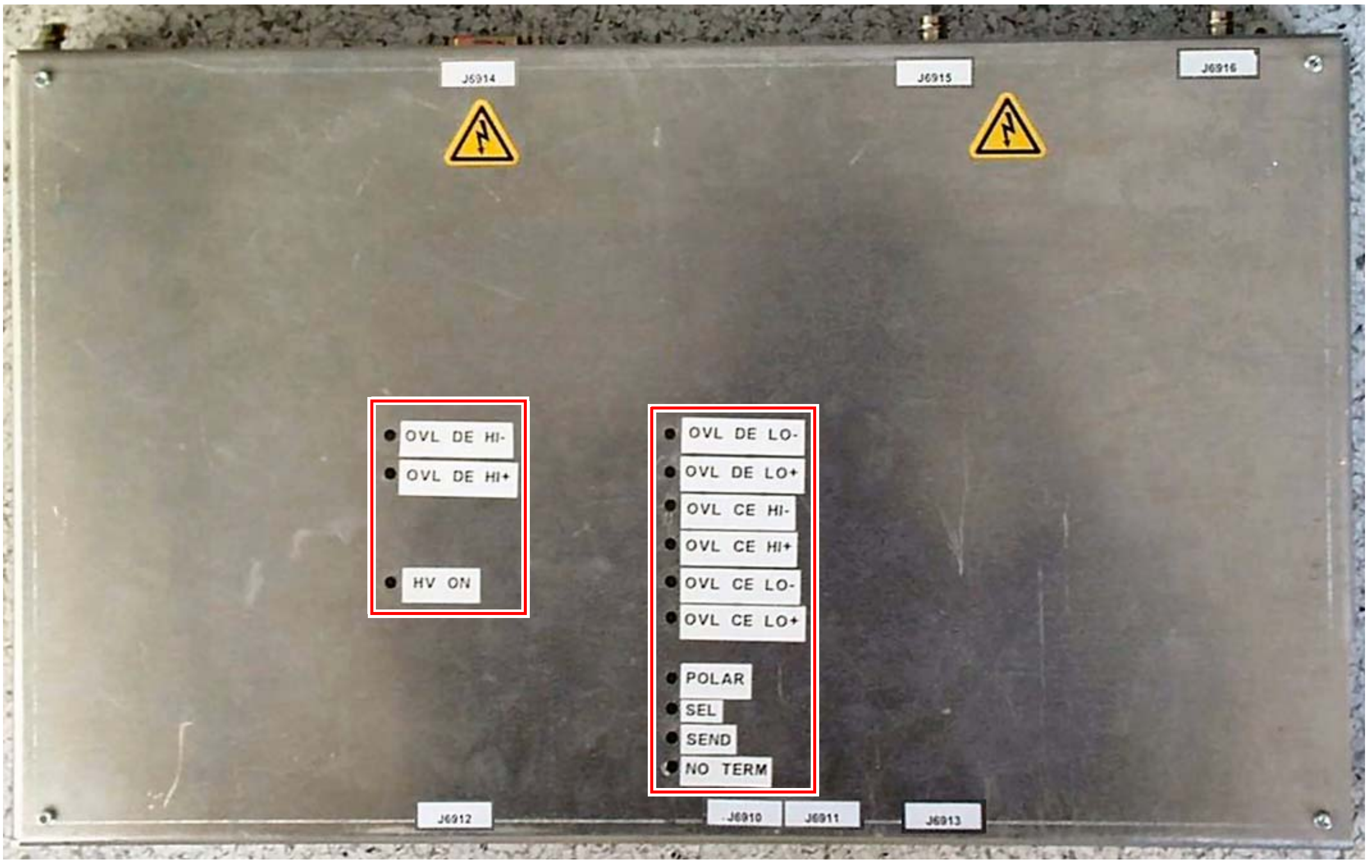

Figure 1-37. Central Electrode Power Supply board

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 1-17 show the status of the voltages applied to the board as well as some operating states. The position of the LEDs on the board is indicated by the red rectangles in Figure 1-37 on page 1-52.

Table 1-17. 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 1-32 on page 1-45. This board provides five dc voltages for the ion optics of the Product Short Name. Two voltages supply the lenses of the instrument. Three voltages are applied to the RF CLT main board to be used as

[1]Part number of complete unit.

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! ▲

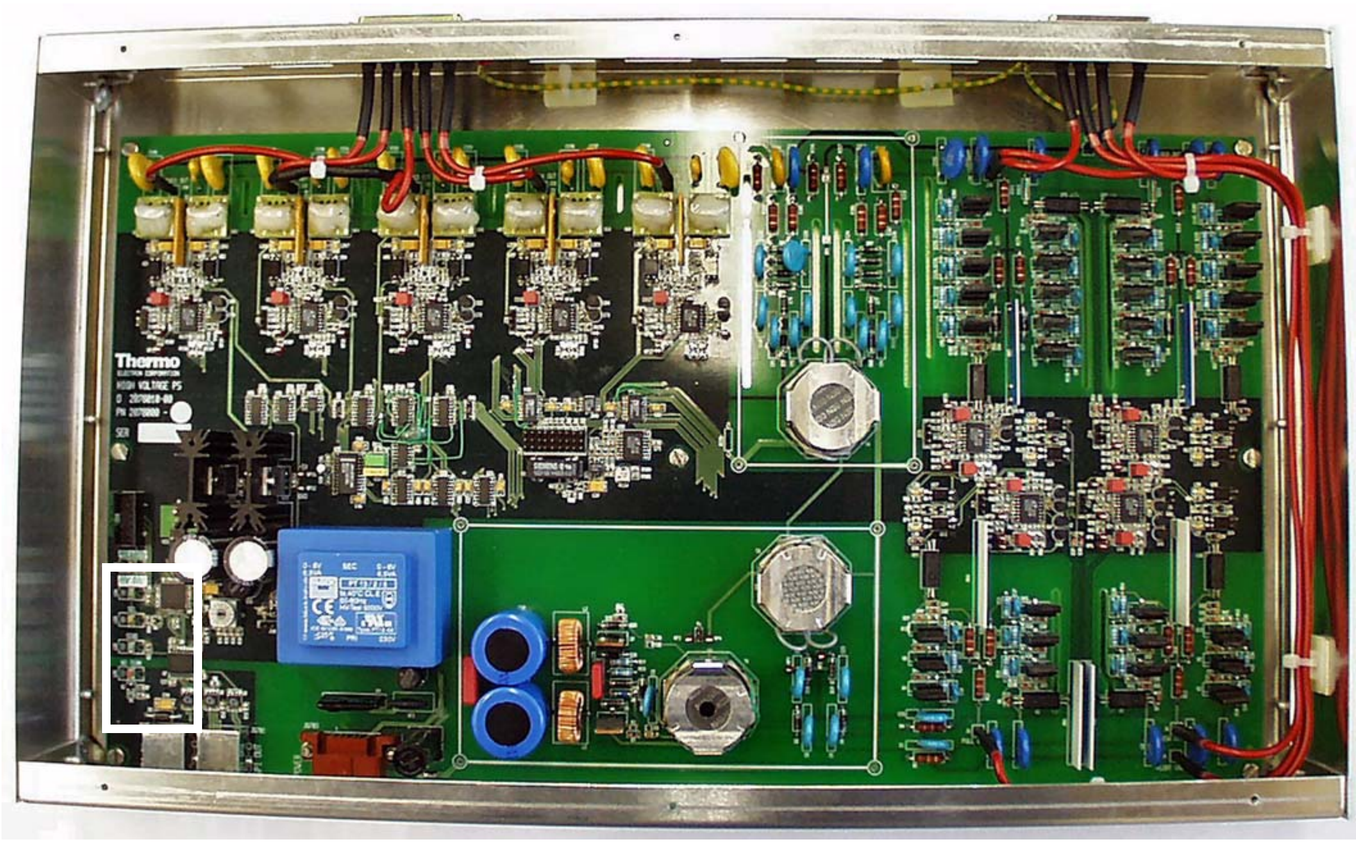

Figure 1-38. High Voltage Power Supply board (cover removed)

The diagnostic LEDs listed in Table 1-18 on page 1-55 show the operating states of the board. The position of the LEDs on the board is indicated by a white rectangle in Figure 1-38.

Table 1-18. 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 1-39.

Figure 1-39. High Voltage Power Supply board with SPI Bus Termination board

Chapter 2 Basic System Operations

Many maintenance procedures for the LTQ Orbitrap Discovery system require that the MS detector be shut down. In addition, the LTQ Orbitrap Discovery 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 Discovery) in the Off (O) position. This turns off all power to the instrument, including the linear ion trap, multiple socket outlets for the data system, and the vacuum pumps. The main power switch must be turned 90° anti-clockwise to switch off the instrument. See Figure 2-1.

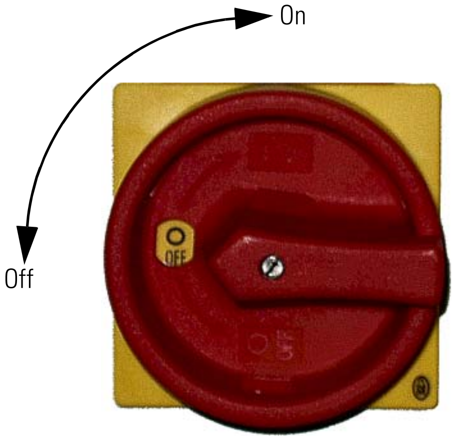

Figure 2-1. Main power switch in Off position

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 System" on page 2-5 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 is started up automatically i.e. the pumps are switched on and the vacuum is created. If the system has been vented during the mains failure, it is necessary to bakeout 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 System in Standby Condition

The LTQ Orbitrap Discovery 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.

Use the following procedure to place the LTQ Orbitrap Discovery system in the Standby condition:

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

2. Turn off the flow of sample solution 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 Discovery main power switch in the On position.

Shutting Down the System

The LTQ Orbitrap Discovery system does not need to be shut down completely if you are not going to use it for a short period of time, such as overnight or over a weekend. Refer to the topic “Placing the System in Standby Condition” on page 2-4. This section describes how to shut down the system for a maintenance or service procedure.

Use the following procedure to shut down the LTQ Orbitrap Discovery system:

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

2. Turn off the flow of sample solution 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 sheath and 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 Discovery in the On position.

7. During service or maintenance operations that require opening the vacuum system of the LTQ XL or LTQ Orbitrap Discovery, 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 before you service them (the ion transfer tube at about 300 °C, for example). ▲

Note If you are planning to perform routine or preventive system maintenance on the LTQ Orbitrap Discovery 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 Discovery 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 software is received from the data system. ▲

Use the following procedure to start up the LTQ Orbitrap Discovery:

1. Start up the (optional) LC and autosampler as is described in the manual that came with the LC and autosampler.

2. Start up the data system and the chiller.

3. Turn on the flows of helium and nitrogen – and argon if present – 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 Discovery 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 octapole 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 3 min, 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 depressed (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. If you do not have either, go to the topic "Setting Up Conditions for Operation" below.

Setting Up Conditions for Operation

Set up your LTQ Orbitrap Discovery for operation, as follows:

1. Before you begin data acquisition with your LTQ Orbitrap Discovery system, you need to allow the system to pump down for at least 8 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 if present: 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. Select the **Display Status View** button in the Tune Plus window. Check to see 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 Discovery Getting Started* manual.

Resetting the System

If communication between the LTQ Orbitrap Discovery 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 Discovery 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 2-7.

To reset the LTQ Orbitrap Discovery, press the Reset button of the linear ion trap. 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 3 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 Discovery 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 Discovery 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. ▲

Chapter 3 User Maintenance

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

Note 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 3 months or if oil is cloudy or discolored	Manufacturer's documentation
Turbomolecular pumps	Exchange lubricant reservoir	Yearly	Manufacturer's documentation page 3-6
Recirculating chiller	Check cooling fluid level Check cooling fluid filter Check air inlet filter	See manufacturer's documentation	Manufacturer's documentation page 3-7

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

- Proceed methodically
- Always wear clean, lint-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 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 Discovery.
- 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. ▲

Baking Out the System

This section provides information and help concerning the system bakeout of the LTQ Orbitrap Discovery. The bakeout procedure removes unwanted gases or molecules (collected or remaining) from the high vacuum region of the instrument. Ions can collide with those gases or molecules resulting in lower overall sensitivity. Therefore, 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 8 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 the section ”Placing the System in Standby Condition” on page 2-4.

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

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.

4. Start the bakeout procedure by pressing the green start button on the right. The LTQ Orbitrap Discovery 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.

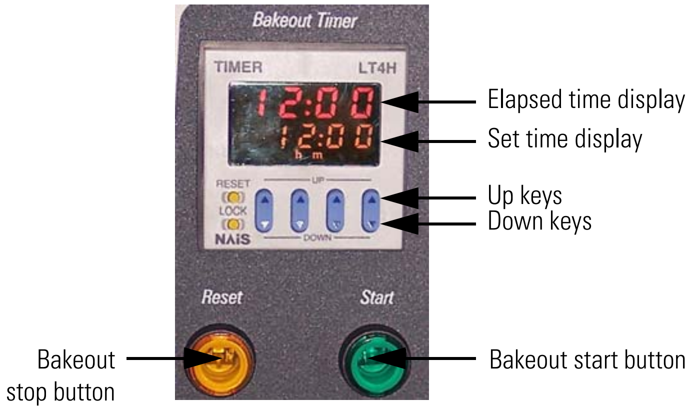

Figure 3-1. Bakeout timer

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 + Vacuum) on the front side that have stopped flashing.

Maintaining the Vacuum System

The turbopumps[1] need maintenance work that is briefly outlined below.

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 in a one-year cycle. 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.

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

Maintenance of the Recirculating Chiller

For the NESLAB ThermoFlex 900 recirculating chiller, the following checks 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 Discovery 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 Discovery / LTQ Orbitrap Discovery Preinstallation Requirements Guide*.

Table 4-1. Parts for the LTQ Orbitrap Discovery

Designation	Part No.
LTQ Orbitrap Discovery; 50 Hz*	072 3720
LTQ Orbitrap Discovery; 60 Hz	072 3730
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
Upgrade kit Orbitrap HCD option†*	122 4800

*Module, for parts list see below.

†Optional equipment.

Table 4-2. Parts LTQ Orbitrap Discovery; 50 Hz (P/N 072 3720)

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
Software 2.4 Tune LTQ Orbitrap Discovery	122 7040
Recirculating chiller Neslab ThermoFlex 900 PD-1 230V/50 Hz†	101161010000004

*Module, for parts list see below.

†Some systems are delivered with NESLAB Merlin M33 recirculating chiller.

Parts Basic System

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

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
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 Discovery	122 5100
0040	1	Upgrade kit gas supply LTQ Orbitrap XL†	122 4820
0050	1	Cable, power distribution/valve	210 0310

*HCD is an option for LTQ Orbitrap Discovery. The feature will be not available if the instrument is not equipped with this option.

†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

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

Pos. No.	Qty.	Designation	Part No.
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
0030	1	Octapole Orbitrap, complete	116 6120
0040	4	Washer; 8.4×15×1.5, stainless steel	047 0860
0050	4	Screw; M8X25, 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 schematic overview of the vacuum system, refer to Figure 1-15 on page 1-19.

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
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 Discovery. For a schematical overview of the gas supply, refer to Figure 1-19 on page 1-25.

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
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 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

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

Pos. No.	Qty.	Designation	Part No.
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
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 schematic overview of the cooling water circuit, refer to Figure 1-22 on page 1-28.

†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 Discovery.

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
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 4-6.

Electronics - Right Panel

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

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	210 1320
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
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 Discovery.

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 Discovery.

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

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

Pos. No.	Qty.	Designation	Part No.
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 Discovery.

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

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

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.

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.

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 air and that has been filtered through a sintered nylon filter. A solenoid-operated valve.

vol volume

w width

W watt

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Numerics

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Thermo Fisher Scientific Inc.
81 Wyman Street
P.O. Box 9046
Waltham, Massachussetts 02454-9046
United States

www.thermo.com