Finnigan™ LTQ™

Hardware Manual

97055-97013 Revision B

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❑ Government lab	❑ Group Manager	❑ Drug Metabolism and Pharmacokinetics
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Finnigan LXQ
Hardware Manual

Revision B
97055-97013

	Strongly Agree	Agree	Disagree	Strongly Disagree
The manual is well organized.	1	2	3	4
The manual is clearly written.	1	2	3	4
The manual contains all of the information I need.	1	2	3	4
The instructions are easy to follow.	1	2	3	4
The instructions are complete.	1	2	3	4
The technical information is easy to understand.	1	2	3	4
The figures are helpful.	1	2	3	4
The index and table of contents helped me find information quickly.	1	2	3	4

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EN 55011	(1998)	EN 61000-4-4	(1995)
EN 61326	(1998)	EN 61000-4-5	(1995)
EN 61000-4-2	(1998)	EN 61000-4-6	(1996)
EN 61000-4-3	(1996)	EN 61000-4-11	(1994)
ENV 50204	(1995)	FCC Class A	

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Notice on Lifting and Handling of Thermo Electron San Jose Instruments

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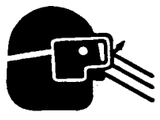
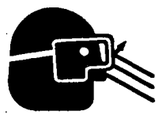
In compliance with international regulations: If this instrument is used in a manner not specified by Thermo Electron San Jose, the protection provided by the instrument could be impaired.

CAUTION Symbol	CAUTION	危険警告	危險警告
	**Electric Shock:** 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 MS detector with the top cover off. Do not remove protective covers from PCBs.	**電撃**：この計測器は高電圧を使用し、人体に危害を与える可能性があります。保守・修理は、必ず操業を停止し、電源を切ってから実施して下さい。上部カバーを外したままで質励分析計の検知機を使用しないで下さい。プリント配線板の保護カバーは外さないで下さい。	電擊：儀器設備使用會造成人身傷害的高伏電壓。在維修之前，必須先關儀器設備並切除電源。務必要在頂蓋蓋上的情況下操作MS檢電器。請勿拆除PCB保護蓋。
	**Chemical:** Hazardous chemicals might be present in the instrument. Wear gloves when handling toxic, carcinogenic, mutagenic, or corrosive/irritant chemicals. Use approved containers and procedures for disposing of waste oil.	**化学物質**：危険な化学物質が計測器中に存在している可能性があります。毒性、発がん性、突然変異性、腐食・刺激性などのある薬品を取り扱う際は、手袋を着用して下さい。廃油の処分には、規定の容器と手順を使用して下さい。	化學品：儀器設備中可能存在有危險性的化學物品。接觸毒性致癌、誘變或腐蝕／刺激性化學品時，請配帶手套。處置廢油時，請使用經過許可的容器和程序。
	**Heat:** Allow heated components to cool before servicing them.	**熱**：熱くなった部品は冷えるのを待ってから保守・修理を行って下さい。	高溫：請先等高溫零件冷卻之後再進行維修。
	**Fire:** Use care when operating the system in the presence of flammable gases.	**火災**：可燃性のガスが存在する場所でシステムを操作する場合は、充分な注意を払って下さい。	火災：在有易燃氣體的場地操作該系統時，請務必小心謹慎。
	**Eye Hazard:** Eye damage could occur from splattered chemicals or flying particles. Wear safety glasses when handling chemicals or servicing the instrument.	**眼に対する危険**：化学物質や微粒子が飛散して眼を傷つける危険性があります。化学物質の取り扱い、あるいは計測器の保守・修理に際しては防護眼鏡を着用して下さい。	眼睛傷害危險：飛濺的化學品或顆粒可能造成眼睛傷害。處理化學品或維儀器設備時請佩戴安全眼鏡。
	**General Hazard:** A hazard is present that is not included in the above categories. Also, this symbol is used on the instrument to refer the user to instructions in this manual.	**一般的な危険**：この標識は上記以外のタイプの危険が存在することを示します。また、計測器にこの標識がついている場合は、本マニュアル中の指示を参照して下さい。	一般性危險：說明未包括在上述類別中的其他危險。此外，儀器設備上使用這個標誌，以指示用戶本使用手冊中的說明。
	When the safety of a procedure is in doubt, before you proceed, contact your local Technical Support Organization for Thermo Electron San Jose Products.	**安全を確保する手順がよくわからない時は、作業を一時中止し、お近くのサーモエレクトロンサンローゼプロダクトのテクニカールサポートセンターごご連絡ください。**	如对安全程序有疑问，请在操作之前与当地的菲尼根技术服务中心联系。

CAUTION Symbol	CAUTION	VORSICHT	ATTENTION	PRECAUCION	AVVERTÉNZA
	**Electric Shock:** 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 MS detector with the top cover off. Do not remove protective covers from PCBs.	**Elektroschock:** In diesem Gerät werden Hochspannungen verwendet, die Verletzungen verursachen können. Vor Wartungsarbeiten muß das Gerät abgeschaltet und vom Netz getrennt werden. Betreiben Sie den MS-Detektor nicht mit abgenommenem Deckel. Nehmen Sie die Schutzabdeckung von Leiterplatten nicht ab.	**Choc électrique** : L'instrument utilise des tensions capables d'infliger des blessures corporelles. L'instrument doit être arrêté et débranché de la source de courant avant toute intervention. Ne pas utiliser le détecteur de SM sans son couvercle. Ne pas enlever les étuis protecteurs des cartes de circuits imprimés.	**Descarga eléctrica**: Este instrumento utiliza altas tensiones, capaces de producir lesiones personales. Antes de dar servicio de mantenimiento al instrumento, éste deberá apagarse y desconectarse de la línea de alimentación eléctrica. No opere el instrumento sin sus cubiertas exteriores instaladas. No remueva las cubiertas protectoras de las tarjetas de circuito impreso.	**Shock da folgorazione.** L'apparecchio è alimentato da corrente ad alta tensione che può provocare lesioni fisiche. Prima di effettuare qualsiasi intervento di manutenzione occorre spegnere ed isolare l'apparecchio dalla linea elettrica. Non attivare il spettrometro di massa (MS) senza lo schermo superiore. Non togliere i coperchi di protezione dalle schede di circuito stampato (PCB).
	**Chemical:** Hazardous chemicals might be present in the instrument. Wear gloves when handling toxic, carcinogenic, mutagenic, or corrosive/irritant chemicals. Use approved containers and procedures for disposing of waste oil.	**Chemikalien:** Dieses Gerät kann gefährliche Chemikalien enthalten. Tragen Sie beim Umgang mit toxischen, karzinogenen, mutagenen oder ätzenden/reizenden Chemikalien Schutzhandschuhe. Entsorgen Sie verbrauchtes Öl entsprechend den Vorschriften in den vorgeschriebenen Behältern.	**Chimique** : Des produits chemiques dangereux peuvent se trouver dans l'instrument. Porter des gants pour manipuler tous produits chemiques toxiques, cancérigènes, mutagènes ou corrosifs/irritants. Utiliser des récipients et des procédures homologuées pour se débarrasser des déchets d'huile.	**Química**: El instrumento puede contener productos químicos peligrosos. Utilice guantes al manejar productos químicos tóxicos, carcinógenos, mutágenos o corrosivos/irritantes. Utilice recipientes y procedimientos aprobados para deshacerse del aceite usado.	**Prodotti chimici.** Possibile presenza di sostanze chimiche pericolose nell'apparecchio. Indossare dei guanti per maneggiare prodotti chimici tossici, cancerogeni, mutageni, o corrosivi/irritanti. Utilizzare contenitori approvo e seguire la procedura indicata per lo smaltimento dei residui di olio.
	**Heat:** Allow heated components to cool before servicing them.	**Hitze:** Warten Sie erhitzte Komponenten erst nachdem diese sich abgekühlt haben.	**Haute température** : Permettre aux composants chauffés de refroidir avant toute intervention.	**Altas temperaturas**: Permita que los componentes se enfríen, antes de efectuar servicio de mantenimiento.	**Calore.** Attendere che i componenti riscaldati si raffreddino prima di effettuare l'intervento di manutenzione.
	**Fire:** Use care when operating the system in the presence of flammable gases.	**Feuer:** Vorsicht, wenn Sie das System in Gegenwart von entzündbaren Gasen betreiben.	**Incendie** : Agir avec précaution lors de l'utilisation du système en présence de gaz inflammables.	**Fuego**: Tenga cuidado al operar el sistema en presencia de gases inflamables.	**Incendio.** Adottare le dovute precauzioni quando si usa il sistema in presenza di gas infiammabili.
	**Eye Hazard:** Eye damage could occur from splattered chemicals or flying particles. Wear safety glasses when handling chemicals or servicing the instrument.	**Verletzungsgefahr der Augen:** Verspritzte Chemikalien oder kleine Partikel können Augenverletzungen verursachen. Tragen Sie beim Umgang mit Chemikalien oder bei der Wartung des Gerätes eine Schutzbrille.	**Danger pour les yeux** : Des projections chimiques, liquides ou solides peuvent être dangereuses pour les yeux. Porter des lunettes de protection lors de toute manipulation de produit chimique ou pour toute intervention sur l'instrument.	**Peligro para los ojos**: Las salpicaduras de productos químicos o partículas que salten bruscamente pueden causar lesiones en los ojos. Utilice anteojos protectores al manipular productos químicos o al darle servicio de mantenimiento al instrumento.	**Pericolo per la vista.** Gli schizzi di prodotti chimici o delle particelle presenti nell'aria potrebbero causare danni alla vista. Indossare occhiali protettivi quando si maneggiano prodotti chimici o si effettuano interventi di manutenzione sull'apparecchio.
	**General Hazard:** A hazard is present that is not included in the above categories. Also, this symbol is used on the instrument to refer the user to instructions in this manual.	**Allgemeine Gefahr:** Es besteht eine andere Gefahr, die nicht in den vorstehenden Kategorien beschrieben ist. Dieses Symbol auf dem Gerät weist den Bediener auch auf Anweisungen in diesem Handbuch hin.	**Danger général** : Indique la présence d'un risque n'appartenant pas aux catégories citées plus haut. Ce symbole figure également sur l'instrument pour renvoyer l'utilisateur aux instructions du présent manuel.	**Peligro general**: Significa que existe un peligro no incluido en las categorías anteriores. Este símbolo también se utiliza en el instrumento para referir al usuario a las instrucciones contenidas en este manual.	**Pericolo generico.** Pericolo non compreso tra le precedenti categorie. Questo simbolo è utilizzato inoltre sull'apparecchio per segnalare all'utente di consultare le istruzioni descritte nel presente manuale.
	When the safety of a procedure is in doubt, before you proceed, contact your local Technical Support Organization for Thermo Electron San Jose Products.	Wenn Sie sich über die Sicherheit eines Verfahrens im unklaren sind, setzen Sie sich, bevor Sie fortfahren, mit Ihrer lokalen technischen Unterstützungsorganisation für Thermo Electron San Jose Produkte in Verbindung.	Si la sûreté d'un procédure est incertaine, avant de continuer, contacter le plus proche Service Clientèle pour les produits de Thermo Electron San Jose.	Cuando la certidumbre acerca de un procedimiento sea dudosa, antes de proseguir, pongase en contacto con la Oficina de Asistencia Tecnica local para los productos de Thermo Electron San Jose.	Quando e in dubbio la misura di sicurezza per una procedura, prima di continuare, si prega di mettersi in contatto con il Servizio di Assistenza Tecnica locale per i prodotti di Thermo Electron San Jose.

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Contents

Read This First

Welcome to the Thermo Electron, Finnigan™ LTQ™ system! The LTQ is a member of the Finnigan family of mass spectrometer (MS) detectors.

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

The **Finnigan LTQ Hardware Manual** includes the following chapters:

Chapter 1: Introduction discusses the ion polarity modes, ionization modes, and scan modes of your LTQ system.

Chapter 2: Functional Description describes the principal components of your LTQ system and their respective functions.

Chapter 3: Daily Operation describes the checks and cleaning procedures of the LTQ system that you should perform every day before you begin your first analysis and after your final analysis.

Chapter 4: MS detector Maintenance outlines the maintenance procedures that you should perform on a regular basis to maintain optimum MS detector performance.

Chapter 5: System Shutdown, Startup, and Reset provides procedures for shutting down and starting up the LTQ system.

Chapter 6: Diagnostics and PCB and Assembly Replacement discusses procedures for testing the major electronic circuits within the instrument and for replacing failed PCBs and assemblies.

Chapter 7: Replaceable Parts lists the replaceable parts for the MS detector and data system.

Changes to the Manual and Online Help

To suggest changes to this manual or the online Help, please send your comments to:

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U.S.A.

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

Abbreviations

The following abbreviations are used in this and other manuals and in the online Help.

A	ampere
ac	alternating current
ADC	analog-to-digital converter
AP	acquisition processor
APCI	atmospheric pressure chemical ionization
API	atmospheric pressure ionization
ASCII	American Standard Code for Information Interchange
b	bit
B	byte (8 b)
baud rate	data transmission speed in events per second
°C	degrees Celsius
CD	compact disc
CD-ROM	compact disc read-only memory
cfm	cubic feet per minute
CI	chemical ionization
CIP	carriage and insurance paid to
cm	centimeter
cm^3	cubic centimeter
CPU	central processing unit (of a computer)
CRC	cyclic redundancy check
CRM	consecutive reaction monitoring
<Ctrl>	control key on the terminal keyboard
d	depth
Da	dalton
DAC	digital-to-analog converter
dc	direct current
DDS	direct digital synthesizer
DEP™	direct exposure probe
DS	data system
DSP	digital signal processor

EI	electron ionization
EMBL	European Molecular Biology Laboratory
<Enter>	enter key on the terminal keyboard
ESD	electrostatic discharge
ESI	electrospray ionization
eV	electron volt
f	femto (10^{-15})
°F	degrees Fahrenheit
.fasta file	extension of a SEQUEST search database file
FOB	free on board
ft	foot
FTP	file transfer protocol
g	gram
G	giga (10^{9})
GC	gas chromatograph; gas chromatography
GC/MS	gas chromatograph / MS detector
GND	electrical ground
GPIB	general-purpose interface bus
GUI	graphical user interface
h	hour
h	height
HPLC	high-performance liquid chromatograph
HV	high voltage
Hz	hertz (cycles per second)
ICIS™	Interactive Chemical Information System
ICL™	Instrument Control Language™
ID	inside diameter
IEC	International Electrotechnical Commission
IEEE	Institute of Electrical and Electronics Engineers
in.	inch
I/O	input/output
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	liquid chromatograph; liquid chromatography
LC/MS	liquid chromatograph / MS detector
LED	light-emitting diode
µ	micro (10^{-6})
m	meter
m	milli (10^{-3})
M	mega (10^{6})
M+	molecular ion
MB	Megabyte (1048576 bytes)
MH+	protonated molecular ion
min	minute
mL	milliliter
mm	millimeter
MS	MS detector; mass spectrometry
MS	MS^n power: where n = 1
MS/MS	MS^n power: where n = 2
MS^n	MS^n power: where n = 1 through 10
m/z	mass-to-charge ratio
n	nano (10^{-9})
NCBI	National Center for Biotechnology Information (USA)
NIST	National Institute of Standards and Technology (USA)
OD	outside diameter
Ω	ohm
p	pico (10^{-12})
Pa	pascal
PCB	printed circuit board
PID	proportional / integral / differential
P/N	part number
P/P	peak-to-peak voltage

ppm	parts per million
psig	pounds per square inch, gauge
RAM	random access memory
RF	radio frequency
RMS	root mean square
ROM	read-only memory
RS-232	industry standard for serial communications
s	second
SIM	selected ion monitoring
solids probe	direct insertion probe
SRM	selected reaction monitoring
SSQ®	single stage quadrupole
TCP/IP	transmission control protocol / Internet protocol
TIC	total ion current
Torr	torr
TSQ®	triple stage quadrupole
u	atomic mass unit
URL	uniform resource locator
V	volt
V ac	volts alternating current
V dc	volts direct current
vol	volume
w	width
W	watt
WWW	World Wide Web

Note. Exponents are written as superscripts. In the corresponding online Help, exponents are sometimes written with a caret (^) or with *e* notation because of design constraints in the online Help. For example:

MS^n (in this manual) MS^n (in the online Help)

10^5 (in this manual) 10^5 (in the online Help)

Typographical Conventions

Typographical conventions have been established for Thermo Electron San Jose manuals for the following:

- Data input
- Boxed information
- Topic headings

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 represented in **bold face letters**. (Titles of topics, chapters, and manuals also appear in bold face letters.)
- 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 and a different font. For example, "click on **Close**".

Boxed Information

Information that is important, but not part of the main flow of text, is displayed in a box such as the one below.

> **Note**. Boxes such as this are used to display information.

Boxed information can be of the following types:

- **Note** – information that can affect the quality of your data. In addition, notes often contain information that you might need if you are having trouble.
- **Tip** – helpful information that can make a task easier.
- **Important** – critical information that can affect the quality of your data.
- **Caution** – information necessary to protect your instrument from damage.
- **CAUTION** – hazards to human beings. Each CAUTION is accompanied by a CAUTION symbol. Each hardware manual has a blue CAUTION sheet that lists the CAUTION symbols and their meanings.
- **DANGER** – laser-related hazards to human beings. It includes information specific to the class of laser involved. Each DANGER is accompanied by the international laser radiation symbol.

Topic Headings

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

Chapter 1
Chapter Name

1.2 Second Level Topics

Third Level Topics

Fourth Level Topics

Fifth Level Topics

Safety Precautions

Observe the following safety precautions when you operate or perform service on the MS detector.

Do Not Perform Any Servicing Other Than That Contained in the Finnigan LTQ Hardware Manual.

To avoid personal injury or damage to the instrument, do not perform any servicing other than that contained in the **Finnigan LTQ Hardware Manual** or related manuals unless you are qualified to do so.

Shut Down the MS Detector and Disconnect It From Line Power Before You Service It.

High voltages capable of causing personal injury are used in the instrument. Some maintenance procedures require that the MS detector be shut down and disconnected from line power before service is performed. Do not operate the MS detector with the top or side covers off. Do not remove protective covers from PCBs.

Respect Heated Zones.

Treat heated zones with respect. The ion transfer capillary and the APCI vaporizer might be very hot and might cause severe burns if they are touched. Allow heated components to cool before you service them.

Place the MS Detector in Standby (or Off) Before You Open the Atmospheric Pressure Ionization (API) Source.

The presence of atmospheric oxygen in the API source when the MS detector is On could be unsafe. (LTQ automatically turns the MS detector Off when you open the API source; however, it is best to take this added precaution.)

Make Sure You Have Sufficient Nitrogen For Your API Source.

Before you begin normal operation each day, make sure that you have sufficient nitrogen for your API source. The presence of atmospheric oxygen in the API source when the MS detector is On could be unsafe. (LTQ automatically turns the MS detector Off when you run out of nitrogen, however, it is best to take this added precaution.)

Provide an Adequate Fume Exhaust System and Contain Waste Streams.

It is your responsibility to provide an adequate fume exhaust system. Samples and solvents that are introduced into the LTQ will eventually be exhausted from the forepump. Therefore, the forepump should be connected to a fume exhaust system. Consult local regulations for the proper method of exhausting the fumes from your system.

The API source can accommodate high flow rates. Therefore, provisions must be made to collect the waste solvent. The API source is fitted with a 6 mm (0.25 in.) ID connector for solvent drainage. A 6 mm (0.25 in.) PVC drain tube, which is provided with the system, should be connected between the API source and an appropriate collection container. (The waste container can be something as simple as an old solvent bottle with a modified cap.)

Do **not** vent the PVC drain tube (or any vent tubing connected to the waste container) to the same fume exhaust system to which you have connected the forepump. The analyzer optics can become contaminated if the API source drain tube and the (blue) forepump exhaust tubing are connected to the same fume exhaust system.

Your laboratory must be equipped with at least two fume exhaust systems. Route the (blue) forepump exhaust tubing to a dedicated fume exhaust system. Route the PVC drain tube from the API source to the waste container. Vent the waste container to a dedicated fume exhaust system.

Use Care When Changing Vacuum Pump Oil.

Treat drained vacuum pump oil and pump oil reservoirs with care. Hazardous compounds introduced into the system might have become dissolved in the pump oil. Always use approved containers and procedures for disposing of waste oil. Whenever a pump that has been operating on a system used for the analysis of toxic, carcinogenic, mutagenic, or corrosive/irritant chemicals, the pump must be decontaminated by the user and certified to be free of contamination before repairs or adjustments are made by a Thermo Electron San Jose Customer Support Engineer or before it is sent back to the factory for service.

Solvent and Gas Purity Requirements

Use the highest purity solvents available. The LTQ MS detector is extremely sensitive to solvent impurities. Some solvent impurities are transparent to UV/Visible detectors, but are easily detected by the LTQ MS detector. Liquid chromatography grade is the minimum acceptable purity. Higher grade solvents are preferred. Distilled water is recommended. Deionized water contains chemicals and is not recommended.

The following is a list of international sources that can supply high quality solvents:

Solvent Source	**Telephone Number**
Mallinckrodt/Baker, Inc.	Tel: (800) 582-2537 Fax: (908) 859-9370
Burdick & Jackson, Inc.	Tel: (800) 368-0050 Fax: (616) 725-6216
E. M. Science, Inc.	Tel: (800) 222-0342 Fax: (800) 336-4422

The LTQ MS detector uses helium as a collision gas. The helium should be high purity (99.995%). The required gas pressure is 135 ± 70 kPa (20 ± 10 psig). Thermo Electron has found that particulate filters are often contaminated and are therefore not recommended.

The LTQ MS detector uses nitrogen as a sheath gas and auxiliary gas. The nitrogen should be high purity (99%). The required gas pressure is 690 ± 140 kPa (100 ± 20 PSI).

Service Philosophy

Servicing the LTQ system consists of performing procedures required to maintain system performance standards, to prevent system failure, and/or to restore the system to an operating condition. Routine and preventive maintenance procedures are documented in this manual.

Routine and preventive maintenance are the responsibility of the user during and after the warranty period. Regular maintenance will increase the life of the system, maximize the up-time of your system, and allow you to achieve optimum system performance.

Service not described in this manual should be performed only by a Thermo Electron Customer Support Engineer or similarly trained and qualified technical personnel.

Level of Repair

Thermo Electron's service philosophy for the LTQ system calls for troubleshooting to the lowest part, assembly, PCB, or module listed in the **Replaceable Parts** chapter of this manual.

For mechanical failures: A mechanical assembly typically is to be repaired to the level of the smallest item listed in the **Replaceable Parts** chapter of this manual.

For electronic failures: PCBs are not repaired to the component level except in certain cases of fuses, relays, etc. When these exceptions occur, the components can be found in the **Replaceable Parts** chapter.

Reply Cards

Thermo Electron San Jose manuals contain one or two reply cards. All manuals contain a Customer Registration / Reader Survey card and some contain a Change of Location card. These cards are located at the front of each manual.

The Customer Registration / Reader Survey card has two functions. First, when you return the card, you are placed on the Thermo Electron San Jose mailing list. As a member of this list, you receive application reports and technical reports in your area of interest, and you are notified of events of interest, such as user meetings. Second, it allows you to tell us what you like and do not like about the manual.

The Change of Location card allows us to track the whereabouts of the instrument. Fill out and return the card if you move the instrument to another site within your company or if you sell the instrument. Occasionally, we need to notify owners of our products about safety or other issues.

Chapter 1
Introduction

The LTQ™ is a member of the Finnigan™ family of mass spectrometer (MS) detectors. The Finnigan LTQ is an advanced analytical instrument that includes a syringe pump, a divert/inject valve, an MS detector, and the Xcalibur® data system. In a typical analysis, a sample can be introduced in any of the following ways:

- Using the syringe pump (direct infusion)
- Using the divert/inject valve fitted with a sample loop and LC (flow injection analysis)
- Using the divert/inject valve and HPLC fitted with a column (LC/MS)

In analysis by LC/MS, a sample is injected onto an LC column. The sample is then separated into its various components. The components elute from the LC column and pass into the MS detector where they are analyzed. Analysis by direct infusion or flow injection provides no chromatographic separation of components in the sample before it passes into the MS detector. The data from the MS detector are then stored and processed by the data system.

Figure 1-1. Finnigan LTQ system

The LTQ MS detector consists of an atmospheric pressure ionization (API) source, ion optics, mass analyzer, and ion detection system. The ion optics, mass analyzer, ion detection system, and part of the API source are enclosed in a vacuum manifold. Ionization of the sample takes place in the API source. The specific method used to ionize the sample is referred to as the ***ionization technique.*** The ions produced in the API source are transmitted by the ion optics into the mass analyzer, where they are trapped in stable orbits by a time-varying electric field. The polarity of the potentials applied to the API source and ion optics determines whether positively charged ions or negatively charged ions are transmitted to the mass analyzer. You can configure the LTQ to analyze positively or negatively charged ions (called the positive or negative ***ion polarity mode***).

The lenses in the API source and ion optics act as a gate to start and stop the transmission of ions from the API source to the mass analyzer. The function of these lenses is controlled by an automatic gain control (AGC) that sets them to transmit the optimum number of ions to the mass analyzer.

The mass-to-charge ratios of the ions produced in the API source are measured by the mass analyzer. Selected ions are ejected from the mass analyzer and reach the ion detection system where they produce a signal. The signal produced is then amplified by the detection system electronics.

The ion detection system signal is analyzed by the LTQ data system. The data system serves as the user interface to the MS detector, autosampler, LC, and syringe pump. Refer to the online Help for more information on the LTQ data processing and instrument control software.

Each sequence of loading the mass analyzer with ions followed by mass analysis of the ions is called a ***scan***. The LTQ uses several different ***scan modes*** and different ***scan types*** to load, fragment, and eject ions from the mass analyzer. The ability to vary the scan mode and scan type, as well as the ionization and ion polarity modes, affords the user great flexibility in the instrumentation for solving complex analytical problems.

This chapter provides an overview of the LTQ. Specific topics covered are as follows:

- Ion polarity modes
- Ionization techniques
- Scan modes
- Scan types
- Data types
- Experiment types

1.1 Ion Polarity Modes

You can operate the LTQ in either of two ***ion polarity modes***: positive or negative. The LTQ can control whether positive ions or negative ions are transmitted to the mass analyzer for mass analysis by changing the polarity of the potentials applied to the API source and ion optics. The ion optics are located between the API source and the mass analyzer.

The information obtained from a positive-ion mass spectrum is different from and complementary to that obtained from a negative-ion spectrum. Thus, the ability to obtain both positive-ion and negative-ion mass spectra aids you in the qualitative analysis of your sample. You can choose the ion polarity mode and ionization technique to obtain maximum sensitivity for the particular analysis of interest.

1.2 Ionization Techniques

You can operate the LTQ using any of four ionization techniques, as follows:

- Electrospray ionization (ESI)
- Atmospheric pressure chemical ionization (APCI)
- Atmospheric pressure photoionization (APPI)
- Nanospray ionization (NSI)

Note. Because APCI, ESI, APPI, and NSI use the same ion source interface (that is, the portion of the API source that is under vacuum), you can switch between these three ionization techniques in just a few minutes. Switching ionization techniques merely involves switching the probes and does not break vacuum.

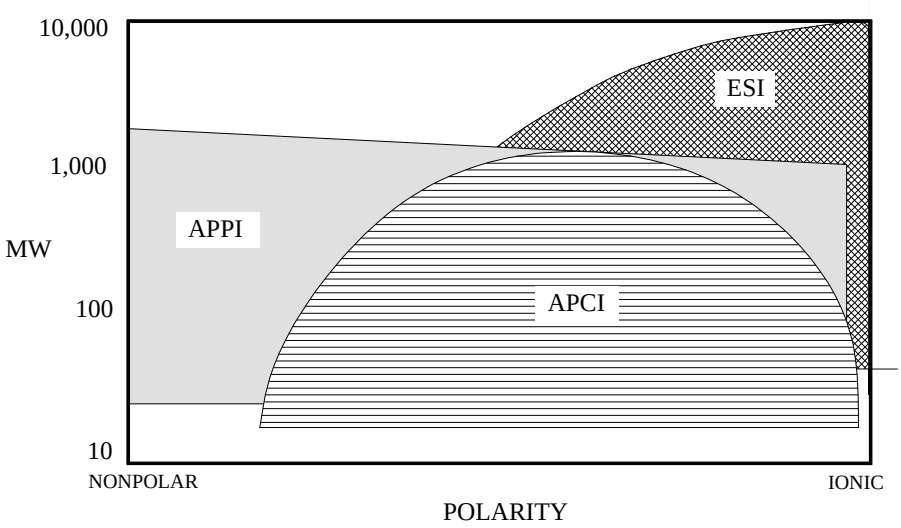


Figure 1-2. Ranges of applicability of APPI, APCI, and ESI

Electrospray Ionization

The electrospray ionization (ESI) technique transforms ions in solution into ions in the gas phase[1]. Many samples that previously were not suitable for mass analysis (for example, heat-labile compounds or high molecular weight compounds) can be analyzed by the use of ESI. ESI can be used to analyze

[1] Refer to the following papers for more information on the electrospray ionization process: Fenn, J. B.; Mann, M.; Meng, C. K.; Wong, S. F.; Whitehouse, C. M. *Mass Spectrom. Reviews* **1990**, *9*, 37; Smith, R. D.; Loo, J. A.; Edmonds, C. G.; Barinaga, C. J.; Udseth, H. R. *Anal. Chem.* **1990**, *62*, 882; Ikonomou, M. G.; Blades, A. T.; Kebarle, P. *Anal. Chem.* **1991**, *63*, 1989.

any polar compound that makes a preformed ion in solution. The term *preformed ion* can include adduct ions. For example, polyethylene glycols can be analyzed from a solution containing ammonium acetate, because of adduct formation between the NH_4^+ ions in the solution and oxygen atoms in the polymer. With ESI, the range of molecular weights that can be analyzed by the LTQ is greater than 100,000 u, due to multiple charging. ESI is especially useful for the mass analysis of polar compounds, which include: biological polymers (for example, proteins, peptides, glycoproteins, and nucleotides); pharmaceuticals and their metabolites; and industrial polymers (for example, polyethylene glycols).

In ESI, ions are produced and analyzed as follows:

1. The sample solution enters the ESI needle, to which a high voltage is applied.
2. The ESI needle sprays the sample solution into a fine mist of droplets that are electrically charged at their surface.
3. The electrical charge density at the surface of the droplets increases as solvent evaporates from the droplets.
4. The electrical charge density at the surface of the droplets increases to a critical point, known as the Rayleigh stability limit. At this critical point, the droplets divide into smaller droplets because the electrostatic repulsion is greater than the surface tension. The process is repeated many times to form very small droplets.
5. From the very small, highly charged droplets, sample ions are ejected into the gas phase by electrostatic repulsion.
6. The sample ions pass through an ion transfer capillary, enter the MS detector and are analyzed.

In the LTQ, the ESI needle is orthogonal to the axis of the ion transfer capillary that carries ions to the MS detector. This geometry keeps the ion transfer capillary clean. The ion sweep cone serves as a mechanical barrier that keeps large droplets and particulates from entering the ion transfer capillary. Figure 1-3 shows the steps in the formation of ions from highly charged droplets, and the relationship between the ESI probe and the ion transfer capillary.

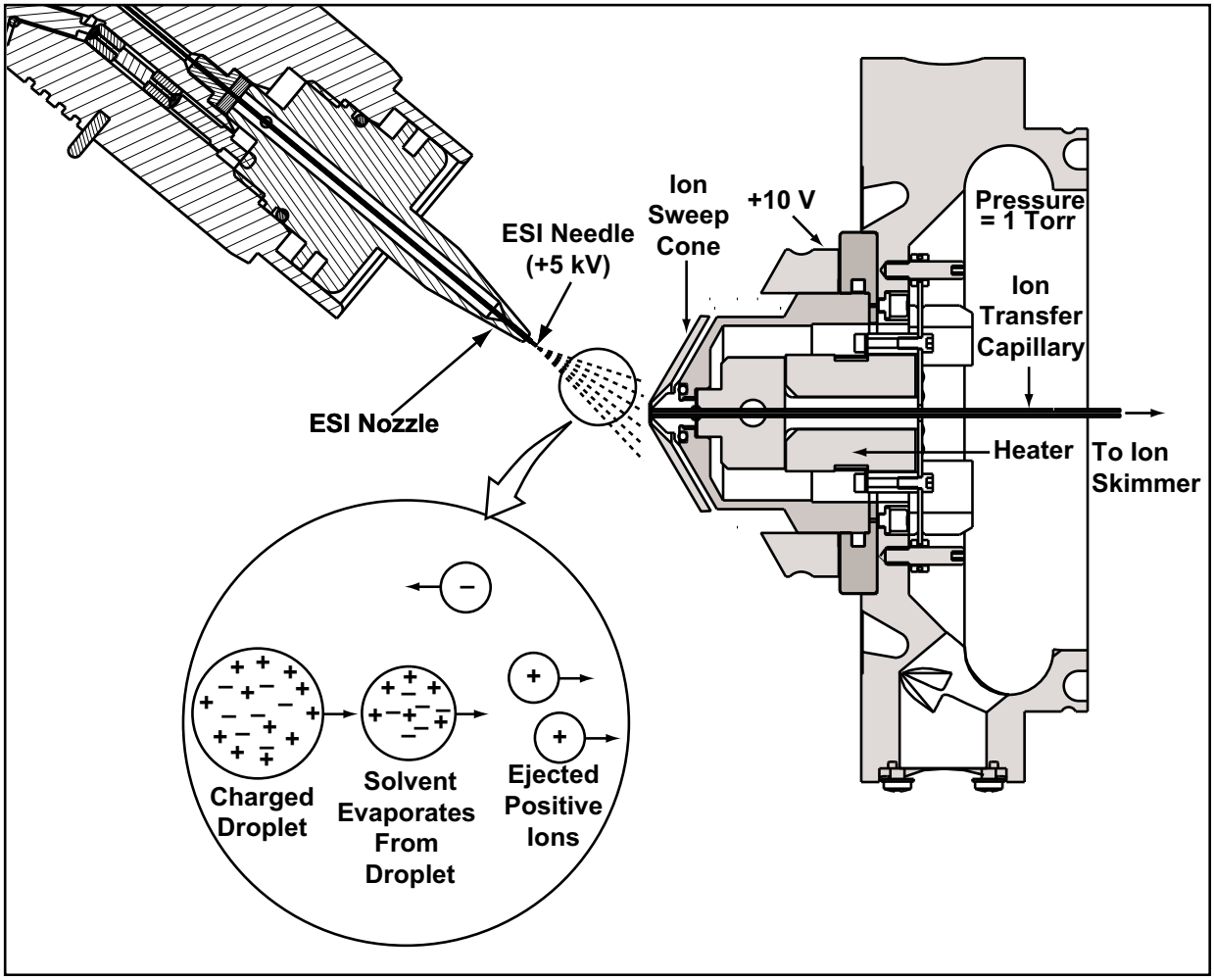


Figure 1-3. ESI process in the positive ion polarity mode

You can use the ESI probe in either positive or negative ion polarity mode. The ion polarity mode of choice is determined by the polarity of the preformed ions in solution: Acidic molecules form negative ions in solution, and basic molecules form positive ions. The ejection of sample ions from droplets is facilitated if the ionic charge and surface charge of the droplet are of the same polarity. Thus, a positively charged needle is used to analyze positive ions and a negatively charged needle is used to analyze negative ions.

Sample ions can carry a single charge or multiple charges. The number of charges carried by the sample ions depends on the structure of the analyte of interest and the carrier solvent. (In ESI, the buffer and the buffer strength both have a noticeable effect on sensitivity. Therefore, it is important to choose these variables correctly.) In the case of higher molecular weight proteins or peptides, the resulting mass spectrum consists typically of a series of peaks corresponding to a distribution of multiply charged analyte ions.

The ESI process is affected by droplet size, surface charge, liquid surface tension, solvent volatility, and ion solvation strength. Large droplets with high surface tension, low volatility, strong ion solvation, low surface charge, and high conductivity prevent good electrospray.

Organic solvents such as methanol, acetonitrile, and isopropyl alcohol are superior to water for ESI. Volatile acids such as acetic acid (1% vol/vol) and formic acid (0.1% vol/vol) and volatile bases such as ammonium hydroxide and triethanolamine are good. Use volatile salts such as ammonium acetate or ammonium formate at concentrations below 10 mM. Strong acids and bases, mineral acids, and nonvolatile salts (such as those containing potassium or sodium) are detrimental.

The rules for a good electrospray are:

- Keep salts out of the solvent system.
- Use the lowest possible HPLC flow rates.
- Use organic/aqueous solvent systems and volatile acids and bases.
- Optimize the pH of the solvent system.

Atmospheric Pressure Chemical Ionization

Atmospheric pressure chemical ionization (APCI) is a soft ionization technique. APCI is used to analyze nonpolar compounds and compounds of medium polarity that are relatively low in molecular weight and have some volatility.

In APCI, ions are produced and analyzed as follows:

1. The APCI nozzle sprays the sample solution into a fine mist of droplets.
2. The droplets are vaporized in a high temperature tube (the vaporizer).
3. A high voltage is applied to a needle located near the exit end of the tube. The high voltage creates a corona discharge that forms reagent ions through a series of chemical reactions with solvent molecules and nitrogen sheath gas.
4. The reagent ions react with sample molecules to form sample ions.
5. The sample ions pass through an ion transfer capillary, enter the MS detector, and are analyzed.

In the LTQ, the sample tube in the APCI nozzle is orthogonal to the axis of the ion transfer capillary that carries ions to the MS detector. This geometry keeps the ion transfer capillary clean. The ion sweep cone serves as a mechanical barrier that keeps large droplets and particulates from entering the ion transfer capillary.

APCI is a gas phase ionization technique. Therefore, the gas phase acidities and basicities of the analyte and solvent vapor play an important role in the APCI process.

In the positive-ion mode, sample ionization occurs in a series of reactions that start with the electron-initiated cation formation. Typical examples of primary, secondary, and adduct ion formation are shown below:

Primary ion formation

$e^- + N_2 \rightarrow N_2^{+\cdot} + 2e^-$

Secondary ion formation

$N_2^{+\cdot} + H_2O \rightarrow N_2 + H_2O^{+\cdot}$

$H_2O^{+\cdot} + H_2O \rightarrow H_3O^+ + HO\cdot$

Proton transfer

$H_3O^+ + M \rightarrow (M+H)^+ + H_2O$

In negative-ion mode, $(M-H)^-$ is typically formed by the abstraction of a proton by OH^-.

APCI is typically used to analyze small molecules with molecular weights up to about 2000 u. APCI is a very robust ionization technique. It is not affected by minor changes in most variables such as changes in buffer or buffer strength.

Figure 1-4 shows the APCI process in the positive ion polarity mode.

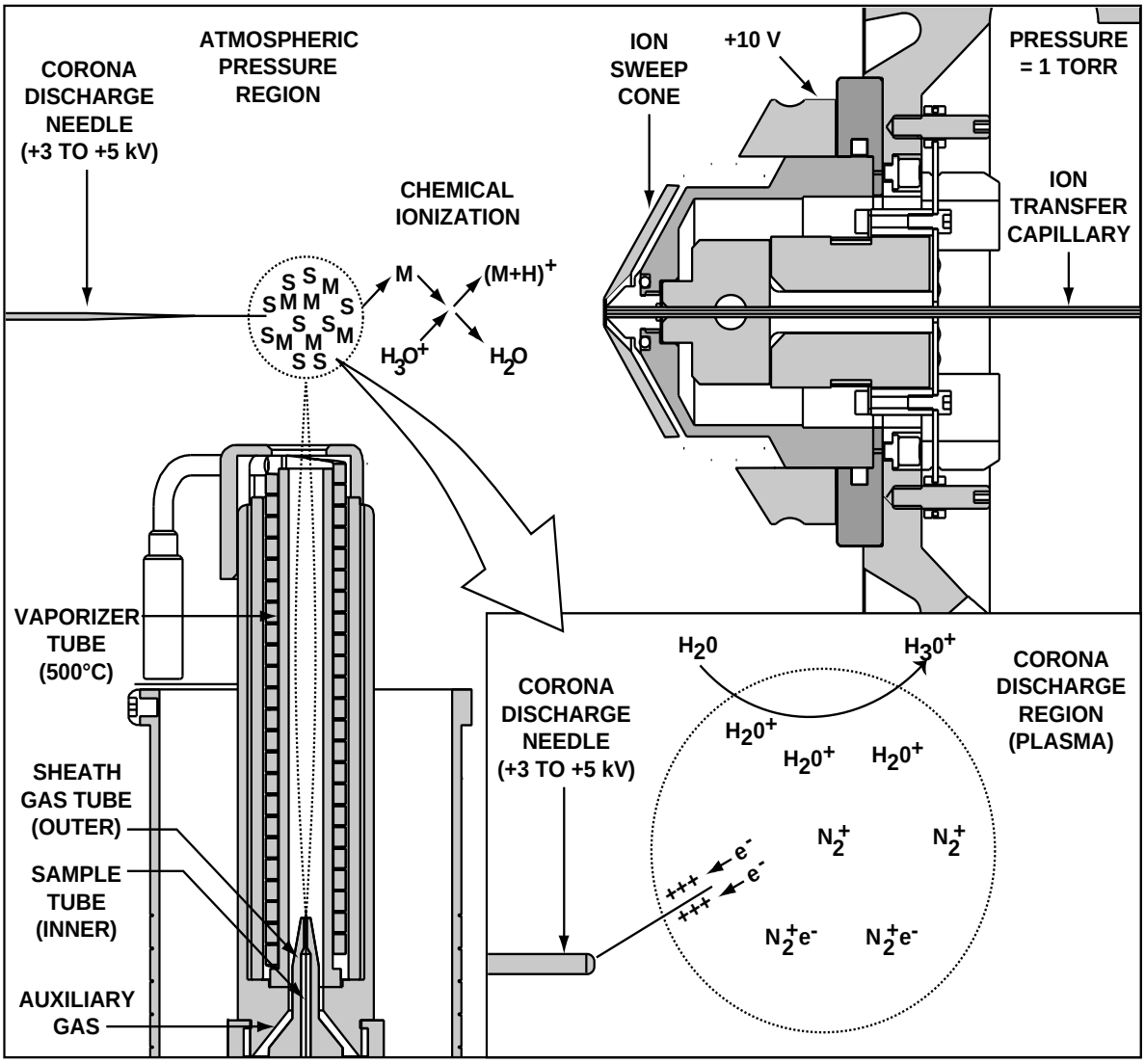


Figure 1-4. APCI process in the positive ion polarity mode

You can use APCI in positive or negative ion polarity mode. For most molecules, the positive-ion mode produces a stronger ion current. This is especially true for molecules with one or more basic nitrogen (or other basic) atoms. An exception to the general rule are molecules with acidic sites such as carboxylic acids and acid alcohols, which produce more negative ions than positive ions.

Although, in general, fewer negative ions are produced than positive ions, negative ion polarity is sometimes the mode of choice. This is because the negative ion polarity mode sometimes generates less chemical noise than does the positive mode. Thus, selectivity might be better in the negative ion mode than in the positive ion mode.

Atmospheric Pressure Photoionization

Atmospheric pressure photoionization (APPI) is also a soft ionization technique. In APPI an ion is generated from a molecule when it interacts with a photon from the Syagen PhotoMate™ light source. APPI generates molecular ions for molecules that have an ionization potential below the photon energy of the light being emitted by the light source.

In APPI, ions are produced and analyzed as follows:

1. The nozzle sprays the sample solution into a fine mist of droplets.
2. The droplets are vaporized in a high temperature tube (the vaporizer).
3. The analyte molecule interacts with the light from the PhotoMate light source. The analyte molecule M is ionized to a molecular ion M^+ if the ionization potential of the analyte is less than the photon energy hν:

   $M + h\nu \rightarrow M^+$
4. In the presence of protic solvents, the analyte ion may extract a hydrogen to form an MH^+ ion:

   $M^+ + S \rightarrow MH^+ + S[-H]$
5. The analyte ions pass through the ion transfer capillary, enter the MS detector, and are analyzed.

Molecules including steroids, basic-drug entities, and pesticides have ionization potentials below the threshold and protonated molecules are generated in the LC/MS experiment. APPI reduces fragmentation because only a small amount of energy is deposited in the molecule. Molecules such as the nitrogen sheath, sweep, and auxiliary gas and the simple solvents used for LC/MS are not ionized because their ionization potentials are greater than the photon energy. The result is selective ionization of analyte vs. background. See Figure 1-5 and Figure 1-6.

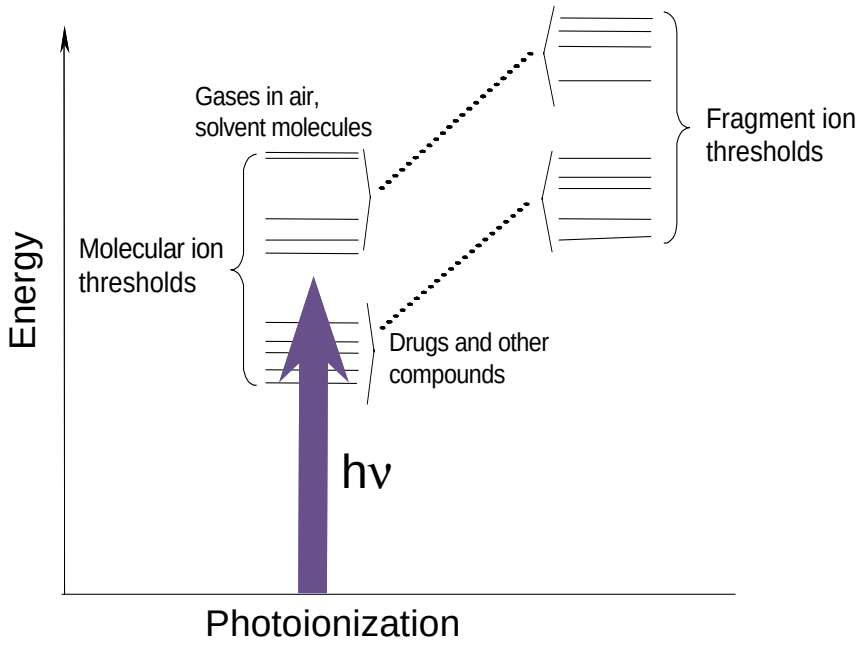


Figure 1-5. Energetics of photoionization

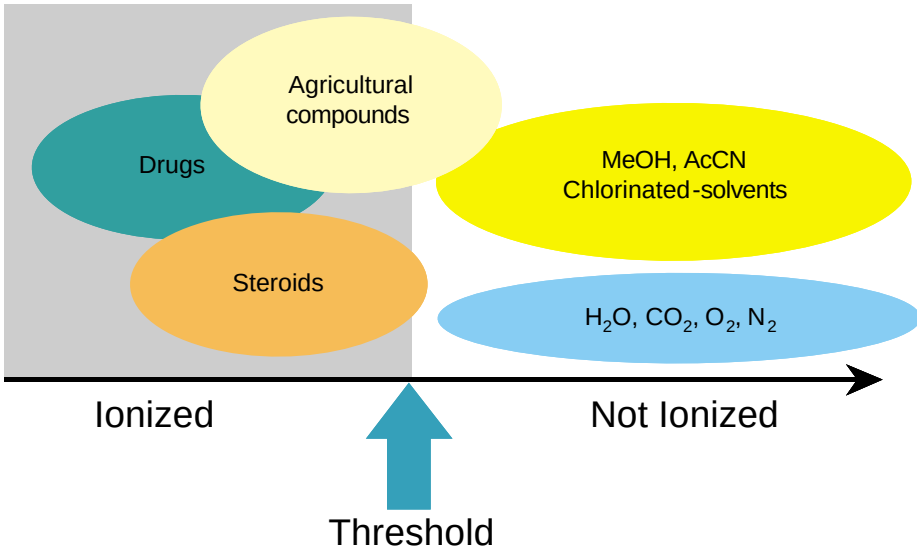


Figure 1-6. Illustration of selective photoionization

The PhotoMate light source uses a krypton lamp which emits photons with energies of 10.0 and 10.6 eV. Molecules with ionization potentials less than 10 eV ionize to form MH^+ while those with greater ionization potentials do not. Figure 1-7 shows ionization potentials of typical compounds and solvents.

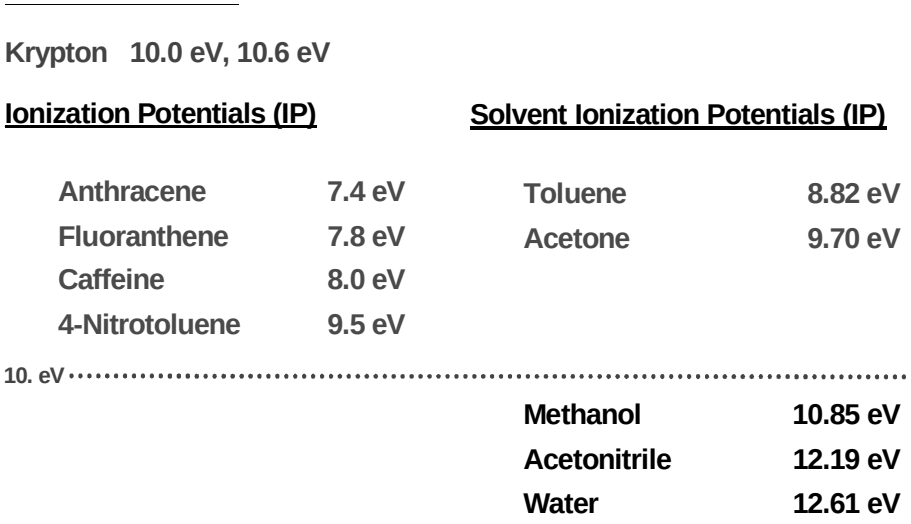


Figure 1-7. Ionization potentials of typical compounds and solvents

Nanospray Ionization

Nanospray ionization (NSI)) is a technique for performing electrospray ionization on amounts of liquid as small as 1 µL for time periods of greater than 30 min. Stable mass spectra can be obtained for very small amounts of biomolecules such as proteins, peptides, oligonucleotides, and oligosaccharides.

For more information on NSI, refer to the manual that came with the NSI source.

1.3 Scan Power and Scan Modes

Ions that are produced in the ion source are often referred to as ***parent ions***. These parent ions can be mass analyzed to produce a mass spectrum. Alternatively, by varying the RF voltages of the mass analyzer, LTQ can first eject all ions except for several selected parent ions, and then collide these ions with helium that is present in the mass analyzer. This helium is known as buffer gas. The collisions of the selected precursor ions with the helium can cause them to fragment into ***product ions***. The product ions can be mass analyzed.

The number of stages of mass analysis is represented as MS^n where *n* is the ***scan power***. (Each stage of mass analysis includes an ion selection step.) LTQ supports scan powers of $n = 1$ and $n = 10$. The higher the scan power, the more structural information is obtained about the analyte.

The scan powers supported by LTQ in its standard configuration are as follows:

- MS scan mode ($n = 1$)
- MS/MS scan mode ($n = 2$)
- MS^n scan mode ($n = 3$ to 10)

MS Scan Mode

The MS or mass spectrometry scan mode corresponds to a single stage of mass analysis (that is, a scan power of n = 1). The MS scan mode involves only parent ions, and no fragmentation of the parent ions takes place. The MS scan mode can be a full scan experiment or a selected ion monitoring (SIM) experiment (see below).

MS/MS Scan Mode

The ***MS/MS scan*** corresponds to two stages of mass analysis ($n = 2$ scan power). In an MS/MS scan, parent ions are fragmented into product ions. An MS/MS scan can be a full scan experiment or a selected reaction monitoring (SRM) experiment (see below).

MS^n Scan Mode

An ***MS^n scan*** involves three to ten stages of mass analysis ($n = 3$ to $n = 10$ scan power). [However, the term can also be applied to one stage of mass analysis (with $n = 1$) or to two stages of mass analysis (with $n = 2$).] An MS^n scan can be either a full scan experiment or a consecutive reaction monitoring (CRM) experiment (see below).

1.4 Scan Types

You can operate the LTQ in the following scan types:

- Full scan
- Selected ion monitoring (SIM)
- Selected reaction monitoring (SRM)
- Consecutive reaction monitoring (CRM)
- ZoomScan™

Full Scan

The ***full scan*** scan type provides a full mass spectrum of each analyte or parent ion. With full scan, in the last step of mass analysis (the ion scan-out step) the mass analyzer is scanned from the first mass to the last mass without interruption.

Full scan scan type provides more information about an analyte than does selected ion monitoring (SIM) or selected reaction monitoring (SRM), but full scan does not provide the sensitivity that can be achieved by the other scan types.

The full scan scan type includes the following:

- Single-stage full scan
- Two-stage full scan

Single-Stage Full Scan

The single-stage full scan type has one stage of mass analysis (n = 1 scan power). With single-stage full scan type, the ions formed in the ion source are stored in the mass analyzer. Then, these ions are sequentially scanned out of the mass analyzer to produce a full mass spectrum.

Single-stage full scan experiments can be used to determine the molecular weight of unknown compounds or the molecular weight of each component in a mixture of unknown compounds. For example, you need a full scan to determine the molecular weight of each component of a mixture of unknown compounds, because you do not know what masses to expect from the mixture.

To use the SIM or SRM scan type, you need to know what ions you are looking for before you can perform an experiment. Thus, for SIM or SRM you can use a full scan to determine the identity of an analyte and obtain its mass spectrum. Then, you might use SIM or SRM to do routine quantitative analysis of the compound.

Two-Stage Full Scan

The two-stage full scan type has two stages of mass analysis (n = 2 scan power). In the first stage of mass analysis, the ions formed in the ion source are stored in the mass analyzer. Then, ions of one mass-to-charge ratio (the parent ions) are selected and all other ions are ejected from the mass analyzer. The parent ions are excited so that they collide with background gas that is present in the mass analyzer. The collisions of the parent ions cause them to fragment to produce one or more product ions.

In the second stage of mass analysis, the product ions are stored in the mass analyzer. Then, they are sequentially scanned out of the mass analyzer to produce a full product ion mass spectrum.

The two-stage full scan type gives you more information about a sample than does SRM, but two-stage full scan type does not yield the speed that can be achieved by SRM. With two-stage full scan, you spend more time monitoring the product ions than you do in SRM. Thus, two-stage full scan provides greater information, but lower speed than SRM does.

To use the SRM scan type, you need to know what parent / product reaction you are looking for before you can perform an experiment. Thus, for SRM you might use one-stage full scan type to determine the parent mass spectrum and two-stage full scan type to determine the product mass spectra for parent ions of interest. Then, you might use SRM to do routine quantitative analysis of the compound.

Selected Ion Monitoring

Selected ion monitoring (SIM) is a single-stage (n = 1 scan power) technique in which a particular ion or set of ions is monitored. In the SIM scan type, the ions formed in the ion source are stored in the mass analyzer. Ions of one or more mass-to-charge ratios are selected and all other ions are ejected from the mass analyzer. Then, the selected ions are sequentially scanned out of the mass analyzer to produce a SIM mass spectrum.

SIM experiments are useful in detecting small quantities of a target compound in a complex mixture when the mass spectrum of the target compound is known. Thus, SIM is useful in trace analysis and in the rapid screening of a large number of samples for a target compound.

Because only a few ions are monitored, SIM can provide lower detection limits and greater speed than a single-stage full scan analysis can provide. SIM achieves lower detection limits because more time is spent monitoring significant ions that are known to occur in the mass spectrum of the target sample. SIM achieves greater speed because only a few ions of interest are monitored; regions of the spectrum that are empty or have no ions of interest are not monitored.

SIM can improve the detection limit and decrease analysis time, but it can also reduce specificity. In SIM, only specific ions are monitored. Therefore, any compound that produces those ions appears to be the target compound. Thus, a false positive result can be obtained.

Selected Reaction Monitoring

Selected reaction monitoring (SRM) is a two-stage (n = 2 scan power) technique in which parent ion and product ion *pairs* are monitored.

In the first stage of mass analysis, the ions formed in the ion source are stored in the mass analyzer. Ions of one mass-to-charge ratio (the parent ions) are selected and all other ions are ejected from the mass analyzer. Then, the parent ions are excited so that they collide with background gas that is present in the mass analyzer. The collisions of the parent ions cause them to fragment to produce one or more product ions.

In the second stage of mass analysis, the product ions are stored in the mass analyzer. Ions of one or more mass-to-charge ratios are selected and all other ions are ejected from the mass analyzer. Then, the selected ions are sequentially scanned out of the mass analyzer to produce an SRM product ion mass spectrum.

Like SIM, SRM allows for the very rapid analysis of trace components in complex mixtures. However, because you are monitoring pairs of ions (one product ion for each parent ion), the specificity obtained in SRM can be much greater than that obtained in SIM. Thus, you are very unlikely to get a false positive result with SRM. To get a false positive result, the interfering compound must do the following: First, it must form a parent ion of the same mass-to-charge ratio as the selected parent ion from the target compound. Second, it must also fragment to form a product ion of the same mass-to-charge ratio as the selected product ion from the target compound.

Consecutive Reaction Monitoring

Consecutive reaction monitoring (CRM) is the multi-stage (n = 3 to n = 10 scan power) analog of SIM (n = 1) and SRM (n = 2), in which a multi-step reaction path is monitored. In the first stage of mass analysis, the ions formed in the ion source are stored in the mass analyzer. Ions of one mass-to-charge ratio (the parent ions) are selected and all other ions are ejected from the mass analyzer. The parent ions are excited so that they collide with background gas that is present in the mass analyzer. The collisions of the parent ions cause them to fragment to produce one or more product ions.

In the second stage of mass analysis, the product ions are stored in the mass analyzer. Product ions of one mass-to-charge ratio are then selected and all other ions are ejected from the mass analyzer. The selected product ions now become the new parent ions for the next stage of mass analysis. The new

parent ions are excited so that they collide with background gas. The collisions of the new parent ions cause them to fragment to produce one or more new product ions.

In the third stage of mass analysis, the new product ions are stored in the mass analyzer. The process described in the previous paragraph is repeated up to seven more times until the final product ions of interest are produced.

In the *n*th stage of mass analysis, the final product ions are stored in the mass analyzer. Ions of one or more mass-to-charge ratios are selected and all other ions are ejected from the mass analyzer. Then, the selected ions are sequentially scanned out of the mass analyzer to produce a CRM final product ion mass spectrum.

In CRM, the specificity increases as the number of consecutive reactions that you monitor increases. However, the sensitivity decreases as the number of consecutive reactions that you monitor increases—especially if there are many fragmentation pathways available to the ion.

ZoomScan

The determination of the mass of an ion from its mass-to-charge ratio may be complicated by the fact that the charge state of the ion may be unknown. ***ZoomScan*** is a high resolution MS scan type in which LTQ performs a high resolution scan that allows you to determine the charge state and molecular weight of an ion. LTQ conducts a high resolution scan of 10 u width and evaluates the ^{12}C /^{13}C isotopic separation of a specified ion or ions. If the isotopic peaks are 1 u apart, the ion has a charge state of ±1. If the isotopic peaks are 0.5 u apart, the ion has a charge state of ±2. If the isotopic peaks are 0.33 u apart, the ion has a charge state of ±3, and so on. You can then determine the molecular weight of the ion from a knowledge of the charge state and mass-to-charge ratio of the ion. You can conduct a ZoomScan analysis of up to ten ions by specifying the mass-to-charge ratios of the ions.

1.5 Data Types

You can acquire and display mass spectral data (intensity versus mass-to-charge ratio) with the LTQ in one of two data types:

- Profile data type
- Centroid data type

Profile Data Type

In the ***profile data type***, you can see the shape of the peaks in the mass spectrum. Each atomic mass unit is divided into approximately 15 sampling intervals. The intensity of the ion current is determined at each of the sampling intervals. The intensity at each sampling interval is displayed with the intensities connected by a continuous line. In general, the profile scan data type is used when you tune and calibrate the MS detector so that you can easily see and measure mass resolution.

Centroid Data Type

In the ***centroid data type***, the mass spectrum is displayed as a bar graph. In this scan data type, the intensities of each set of 15 sampling intervals are summed. This sum is displayed versus the integral center of mass of the 15 sampling intervals. In general, the centroid scan data type is used for data acquisition because the scan speed is faster (but the resolution is lower) and the disk space requirements are smaller. Data processing is also much faster for centroid data.

1.6 Experiment Types

This topic describes several types of experiments that you can perform with the LTQ. The experiments can be grouped into the following categories:

- General MS or MS^n
- Data-Dependent™
- Ion Mapping™
- Ion Tree

You can specify which type of experiment you want to perform in the Instrument Setup window, and then save it in an Instrument Method (*.meth*) file.

> **Note**. Procedures for these experiments are beyond the scope of this **Finnigan LTQ Hardware Manual**. If you need more information, refer to online Help.

General MS or MS^n Experiments

A General MS or MS^n experiment is best used for the quantitative analysis of known compounds. However, you can also use a General experiment to collect qualitative data for structural analysis. Xcalibur includes an Instrument Method template in Instrument Setup so you can get started with a General MS or MS^n experiment.

In a General *MS* quantitation experiment, you need to specify the mass range of your analyte(s) of interest. In a General *MS/MS* quantitation experiment, you need to specify a parent (precursor ion) that fragments into distinctive product ions. In a General MS^n quantitation experiment, you need to specify the mass-to-charge ratios of *all* the parent ions of interest. The LTQ can then collect data on the ions in the range or on the product ions of the parent ion(s) that you specify.

If you use a General experiment to collect data for qualitative (structural) analysis, you specify the scan mode (MS through MS^n) for which you want data in the Scan Event Settings group box. If you specify MS/MS or MS^n, you then choose the parent ion(s) for which you want data in the Set Parent List dialog box. The LTQ can then collect distinct qualitative information for structural analysis or for spectral reference.

The LTQ can generate reproducible, product-specific spectra, even from laboratory to laboratory. Consequently, reference spectra that are generated with the LTQ can be used to confirm structures of compounds generated with other LTQ systems.

Data-Dependent Experiments

A Data-Dependent experiment is best used for the qualitative analysis of unknown compounds for structure elucidation or confirmation. The LTQ uses the information in a Data-Dependent experiment to make decisions about the next step of the experiment automatically — without input from a user. Instrument Setup contains the Instrument Method templates that you need to get started with Data-Dependent experiments.

A Data-Dependent experiment produces a great deal of data from a single sample analysis. You can run a Data-Dependent experiment even if you know very little about your sample, and even if you are unfamiliar with the variables of mass spectroscopy. In a Data-Dependent experiment, you can specify parent ions for fragmentation or you can let the LTQ automatically select the ions for fragmentation. The LTQ can collect the structural information for every parent ion in the sample automatically, even if the sample is a mixture of compounds.

A Data-Dependent experiment requires minimal input from a user about how the experiment should best proceed. The user specifies that one or more scan events of an experiment segment are to be run as Data-Dependent. Then, the LTQ collects MS/MS or MS^n data and makes decisions about what the next step in the experiment should be to collect even more data. For example, in a Data-Dependent Triple Play experiment for a mixture of compounds, the LTQ can decide which parent ion to isolate, the charge state of the parent ion, and the molecular weight of the compound.

Ion Mapping experiments can be Data-Dependent. (The Total Ion Map, Neutral Loss Ion Map, and Parent Ion Map experiments are *not* Data-Dependent.) The Data-Dependent Zoom Map experiment collects ZoomScan data on every scan interval in a specified mass range.

Ion Tree experiments are types of Data-Dependent experiments. These experiments provide methods for automatically interpreting MS^n data and arranging the data in formats that are easy to manipulate.

You can approach the setup of Data-Dependent experiments in either of two ways:

- If you have some idea of the parent ion, or if you expect a certain kind of parent, you can set up a list of possible parent ions. Then, when one of the parent ions you specified is detected, you can acquire product spectra and analyze the information. Conversely, you can also set up a list of ions that you do not want to be selected for fragmentation.
- If you have little information about your compound, you can set up the parameters of a Data-Dependent experiment so that if the intensity of the ion signal is above a specified threshold, the LTQ generates product spectra. Later, you decide if the information is useful. Parameters that you might specify, for example, include threshold values for the intensity of the MS or MS^n ion signal. Whatever threshold values you choose should accomplish the isolation of your parent ions of interest.

You can find useful structural information about your compound automatically with the simplest Data-Dependent experiment, Data-Dependent MS/MS. You specify the MS scan range, and you do not even need to specify a parent ion. The LTQ can then collect full scan MS data, pick the most intense parent ion in the spectrum, and fragment the ion to generate product ions.

A Data-Dependent Triple-Play experiment is the same as Data-Dependent MS/MS, but includes the identification of the charge state of the parent with the LTQ ZoomScan feature. A Data-Dependent Triple-Play experiment collects full scan MS data, and then uses ZoomScan to determine the charge state of the parent ion and calculate the molecular weight. The parent ion is then fragmented into product ions (MS/MS). For example, if the LTQ determines a charge state equal to 2, and if the mass-to-charge ratio of the parent ion is *m/z* 500, then the mass-to-charge ratios of the product ions can be up to *m/z* 1000 (or 2 × 500).

You can use a Data-Dependent experiment (from templates in Instrument Setup) to do the following:

- Identify low-level impurities in high-purity compounds (Data-Dependent MS/MS)
- Identify metabolites in a complex mixture (Chromatographic Separation with Data-Dependent MS/MS)
- Build a custom library of composite MS^n spectra (Ion Tree)

You can use a Data-Dependent MS^n experiment to identify process impurities. In the quality assurance process for aspirin, for example, the LTQ can identify impurities of 0.1%.

A Data-Dependent MS/MS experiment of a complex mixture of drug metabolites can provide highly specific structural information. Characteristic masses along the metabolic pathways of a drug, for example, can produce MS/MS spectra that are specific to the structure of the drug. These spectra are essential in metabolite identification.

A Data-Dependent experiment can produce a composite spectrum of, for example, MS^2, MS^3, and MS^4 data. The LTQ can store the MS^n fingerprint data in a custom MS^n library spectrum. The data is valuable for use in process control, quality assurance, or research.

Ion Mapping Experiments

An Ion Mapping experiment is best used to get full structural characterization of unknown molecules in complex mixtures. In an Ion Mapping experiment, you can get product ion scans on every parent ion over a specified mass range. An Ion Mapping experiment can help to identify automatically which parent ions were fragmented to yield a specified product ion. The experiment “maps” one or more parent ions by using the information from product ion scans.

The LTQ includes the following Ion Mapping templates in Instrument Setup so you can get started with an Ion Mapping experiment:

- Total (or full scan) Ion Map
- Neutral Loss Ion Map
- Parent Ion Map

These Ion Mapping experiments, in general, require that sample solution enter the MS Detector at a composition that is constant throughout. Therefore, you use infusion to introduce your sample for these Ion Mapping experiments.

In a Total (or full scan) Ion Mapping experiment, you get product ion scans for each parent ion, so you can determine which parent ions lost a particular fragment to yield a particular product ion. Furthermore, you can determine which parent ions are related to specific product ions. For example, you can map the spectral peaks in a mass range from *m/z* 400 to *m/z* 2000 and specify to scan for MS/MS product ions in incremental steps of every mass-to-charge ratio, every fifth mass-to-charge ratio, or every tenth mass-to-charge ratio.

A Neutral Loss Ion Mapping experiment collects scans for masses that have lost neutral fragments. As with full scan Ion Mapping, you can get product ion scans on every parent ion. However, a Neutral Loss Ion Map identifies which parent ions lost a neutral fragment of a particular mass. For example, you can specify a neutral loss of 80 u (as in the case of a phosphorylated peptide in a tryptic digest). A Neutral Loss Ion Mapping experiment can step through each product mass in the mixture. The experiment searches for evidence of the loss of a neutral moiety of mass 80 u.

A Parent Ion Mapping experiment identifies all the ions that produce a particular molecular ion that you specify. For example, if you specify a product ion mass of *m/z* 50, a Parent Ion Map includes all the parent ions that yielded the specified product ion, *m/z* 50.

A Data-Dependent Zoom Map is an Ion Mapping experiment that collects ZoomScan data on every scan interval in a mass range that you specify, as well as Data-Dependent MS/MS product spectra on every mass above an intensity threshold.

The results of any of the Ion Mapping experiments can be viewed in the Xcalibur Qual Browser window.

Ion Tree Experiments

In an Ion Tree experiment, the LTQ can collect MS^n data automatically. You can specify a particular parent ion for fragmentation, or you can let the LTQ find the parent ions automatically and fragment them to any level between MS^2 and MS^{10}. The LTQ automates the collection of data by deciding what actions need to occur next for the experiment to progress.

In an Ion Tree experiment, you can specify either of two options that prioritize how the LTQ gathers information: *Depth Focus* and *Breadth Focus.*

- Depth Focus characterizes an ion by performing a series of MS^n-level fragmentations (for example, MS/MS, MS^3, MS^4, etc.) before characterizing the next most intense ion in the MS^n series.
- Breadth Focus characterizes all ions to the same MS^n level before advancing to the next MS^n level.

For example, if you specify a *Maximum Depth* of 3 and a *Maximum Breadth* of 2 in an Ion Tree experiment, the following occurs:

- First, with either Depth or Breadth Focus, the LTQ scans for parent ions (MS) over the specified mass range. The most intense ion of the MS spectrum is selected for fragmentation (MS/MS).
- Second, if you chose the Depth Focus, after the most intense ion of the MS spectrum is fragmented — producing an MS/MS spectrum — the LTQ selects and fragments the most intense ion of the *MS/MS* spectrum. This results in an MS^3 spectrum, the level specified as the maximum depth for this example. The LTQ then backs up one level and fragments the second most intense ion of the *MS/MS* spectrum, creating more product ions on the level of MS^3 from this parent ion. This process is then repeated for the second most intense ion in the *MS* spectrum.
- If you chose the Breadth Focus, after the most intense ion of the MS spectrum is fragmented — producing an MS/MS spectrum — the LTQ selects and fragments the second-most intense ion of the *same* MS spectrum. The fragmentation of parent ions continues to the *Max Breadth* level that you specified (2, for this example). After the two most intense peaks on the MS level are fragmented, the LTQ scans the first *MS/MS* spectrum to select and fragment the two most intense ions. This results in product ions on the level of MS^3, the level specified as the maximum depth for this example. This process is then repeated for the second most intense ion in the *MS* spectrum.

The results of a Data-Dependent Ion Tree experiment can be viewed in the Xcalibur Qual Browser window. The results are displayed as a structure tree that originates from a particular parent ion.

Chapter 2
Functional Description

This chapter describes the principal components of the LTQ system and their respective functions. The principal components of the LTQ system are as follows:

- Autosampler (optional)
- Liquid chromatograph (optional)
- Syringe pump
- Divert/inject valve
- Mass spectrometer (MS) detector
- Data system

A functional block diagram of the LTQ system is shown in Figure 2-1. A sample transfer line connects the LC to the MS detector. The autosampler and LC are usually installed on the left of the MS detector. The syringe pump and divert/inject valve are integrated into the MS detector cabinet.

In a typical analysis, a sample can be introduced in any of the following ways:

- Using the syringe pump (direct infusion)
- Using the divert/inject valve fitted with a loop and an LC (flow injection analysis)
- Using a divert/inject valve and LC fitted with a column (LC/MS)

In analysis by LC/MS, a sample is injected onto an LC column. The sample is then separated into its various components. The components elute from the LC column and pass into the MS detector where they are analyzed.

Upon entering the API source, sample molecules are ionized by electrospray ionization (ESI), atmospheric pressure chemical ionization (APCI), atmospheric pressure photoionization (APPI), or nanospray ionization (NSI). The ion optics focus and accelerate the resulting sample ions into the mass analyzer, where they are analyzed according to their mass-to-charge ratios. The sample ions are then detected by two ion detection systems that produce a signal proportional to the number of ions detected. The ion current signal from the ion detection systems is received and amplified by the system electronics and is then passed on to the data system for further processing, storage, and display. The data system provides the primary LTQ user interface.

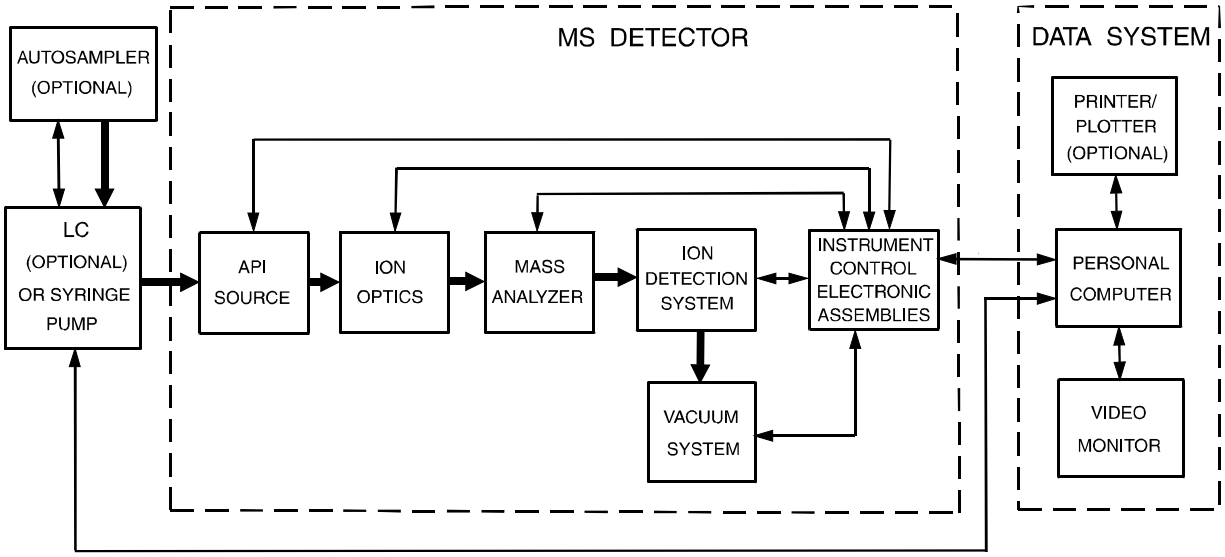


Figure 2-1. Functional block diagram of the LTQ system. The broad, single-headed arrows represent the flow of sample molecules through the instrument. The narrow, double-headed arrows represent electrical connections.

2.1 Autosampler

The ***autosampler*** is used to inject samples automatically into the LC inlet. Thermo Electron (Finnigan Surveyor, AS3000, and AS3500), Waters (2690, 2695, and 2795), and Agilent (1100) autosamplers can be controlled directly from the LTQ data system computer. With an autosampler, you can automate your LC/MS analyses.

> **Note.** For other autosamplers, LTQ provides contact closure Start/Stop signals. Refer to **Finnigan LTQ Getting Connected** for information on connecting an autosampler to the LTQ by contact closure Start/Stop signals.

You can configure the Xcalibur data system for your autosampler from the data system computer. You specify the model name and model number by selecting the appropriate instrument button in the Instrument Configuration window, which is available by choosing **Start > Programs > Xcalibur > Instrument Configuration**. Refer to the Xcalibur online Help for a description of Instrument Configuration.

You can also set up, monitor, and control the autosampler from the data system computer from the Instrument Setup window, which is available by choosing **Start > Programs > Xcalibur > Xcalibur** and then clicking on the Instrument Setup button. Refer to the Xcalibur online Help for a description of Instrument Setup.

Front-panel (keypad) operation of the autosampler and maintenance procedures for the autosampler are described in the documentation provided with the autosampler.

2.2 Liquid Chromatograph

The high performance ***liquid chromatograph*** (LC) separates a sample mixture into its chemical components by liquid chromatography. In liquid chromatography, the sample mixture partitions between a solid stationary phase of large surface area and a liquid mobile phase that percolates over the stationary phase. The molecular structure of each component of the mixture determines when each component elutes from the LC and enters the MS detector.

Thermo Electron (Finnigan Surveyor MS, Surveyor LC, TSP P2000, TSP P4000), and Agilent (1100) LCs (and the corresponding UV detectors) can be controlled directly from the LTQ data system computer. Refer to **Finnigan LTQ Getting Connected** for information on connecting an LC to the LTQ.

You can configure the Xcalibur data system for your LC and UV detector from the data system computer. You specify the model name and model number by selecting the appropriate instrument button in the Instrument Configuration window. Refer to the Xcalibur online Help for a description of Instrument Configuration.

You can also set up, monitor, and control the LC and UV detector from the data system computer from the Instrument Setup window. Refer to the Xcalibur online Help for a description of Instrument Setup.

Front-panel (keypad) operation of the LC and maintenance procedures for the LC are described in the documentation provided with the LC.

2.3 Syringe Pump

The LTQ includes an electronically-controlled, integrated, syringe pump. The ***syringe pump*** delivers sample solution from the syringe into the API source. See Figure 2-2. When the syringe pump is operating, a motor drives a ***pusher block*** that depresses the plunger of the syringe at a rate of 1% of the syringe volume per minute. Liquid flows out of the syringe needle and into the sample transfer line as the plunger is depressed. The syringe is held in place by a ***syringe holder***. Refer to **Finnigan LTQ Getting Started** for instructions on setting up the syringe pump.

You can start and stop the syringe pump from the Syringe Pump dialog box, which can be reached from the Tune Plus window (which is available by choosing **Start > Programs > Xcalibur > LTQ Tune**). You can also specify the Purge mode, in which the flow rate is 5% of the syringe volume per minute. Refer to the Xcalibur online Help for instructions on operating the syringe pump from the data system.

The ***syringe pump LED*** is illuminated green whenever the syringe pump is pumping. The LED is off if the syringe pump is at the end of its travel.

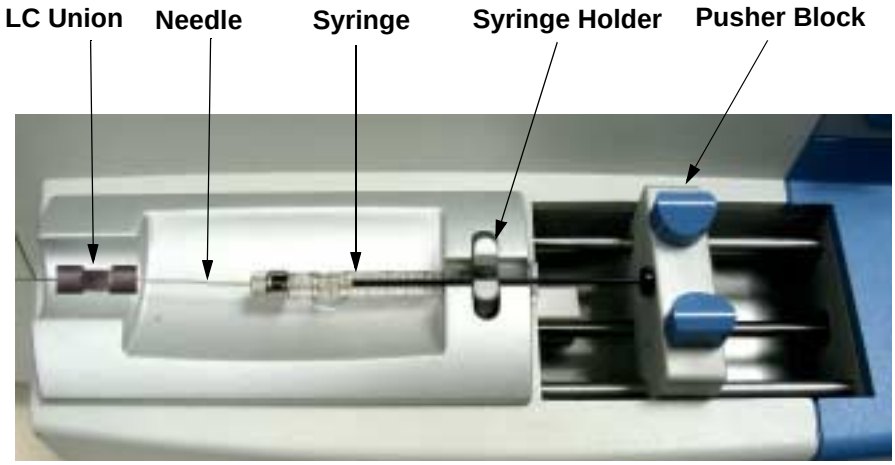


Figure 2-2. Syringe pump

2.4 Divert/Inject Valve

The divert/inject valve is located on the front of the LTQ to the left of the API source. See Figure 2-3. You can configure (plumb) the divert/inject valve as a loop injector (for flow injection analysis) or as a divert valve. Procedures for plumbing the valve in the loop injector or divert valve configuration are given in **Finnigan LTQ Getting Connected**.

You can control the divert/inject valve from the data system. You specify the parameters of the divert/inject valve in the Divert/Inject Valve dialog box, which can be reached from the Tune Plus window, or the Divert Valve page, which can be reached from the Instrument Setup window. Refer to the online Help for instructions on operating the divert/inject valve from the data system.

You can also use the divert/inject valve button to divert the LC flow between the MS detector and waste when the valve is in the divert valve configuration, or switch between load and inject modes when the valve is in the loop injector configuration.

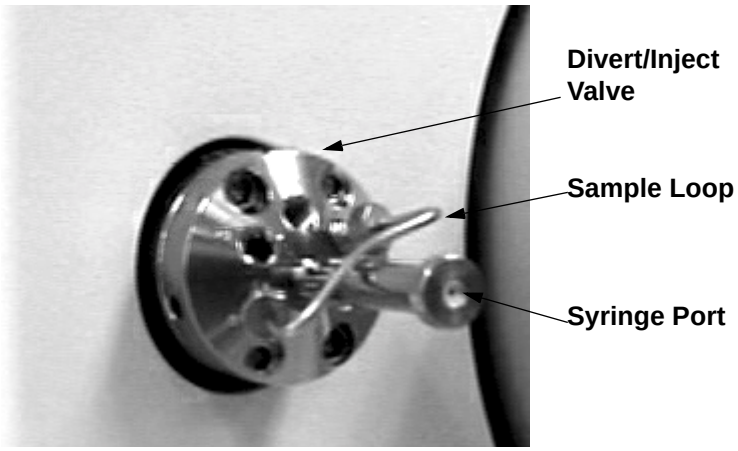


Figure 2-3. Divert/inject valve

2.5 MS Detector

The ***MS detector*** provides sample ionization and mass analysis of injected samples or samples eluted from a liquid chromatograph. The LTQ MS detector uses a linear ion trap mass analyzer with an ion source external to the mass analyzer. Several important features of the LTQ MS detector are as follows:

- Universal, selective, and specific detector
- High sensitivity
- Multiple mass ranges
- ESI, APCI, APPI, and NSI ionization techniques
- Positive and negative ion polarity modes
- MS, MS/MS, and MS^n scan modes
- Full scan, SIM, SRM, CRM, and ZoomScan scan types
- Data-Dependent, Ion Mapping, and Ion Tree experiments

The MS detector includes the following components:

- Controls and indicators
- API source
- Ion optics
- Mass analyzer
- Ion detection system
- Vacuum system and inlet gasses hardware
- Cooling fans
- Electronic assemblies

Controls and Indicators

Five light-emitting diodes (LEDs) are located at the upper right side of the front panel of the MS detector. See Figure 2-4.

The LED labeled *Power* is illuminated whenever power is supplied to the vacuum system and electronic assemblies of the MS detector. The color of the LED depends on whether the MS detector is in the Normal, Warning, or Failure condition, as follows:

- In the Normal condition, the temperature in the MS detector is less than 37 °C and its +5 V dc supply level is between +4.98 and +5.25 V dc. The Power LED is illuminated solid green.

- In the Warning condition, the temperature in the MS detector is marginal, or its +5 V dc is marginal. Marginal temperature is between 37 and 45 °C. Marginal +5 V dc supply level is between +4.75 and 4.97 V dc. The Power LED flashes yellow.
- In the Failure condition, the temperature in the MS detector is greater than 45 °C or its +5 V dc supply level is less than +4.75 V dc. The Power LED is illuminated solid yellow and the MS detector is held in Reset mode until the failure condition is cleared.

The LED labeled *Vacuum* is illuminated green whenever the vacuum protection circuitry indicates that the vacuum is OK and the safety-interlock switch on the API source is depressed (that is, the door on the Ion Max ion source is closed). If the LED labeled Vacuum is not illuminated, high voltage is not applied to LTQ components.

The LED labeled *Communication* is illuminated yellow when the MS detector and the data system are trying to establish a communication link. The Communication LED is illuminated green when the communication link between the MS detector and the data system has been made.

The LED labeled *System* is illuminated yellow whenever the MS detector is in Standby (that is, high voltage is not supplied to the API source, mass analyzer, and ion detection system, but the MS detector power is on). The System LED is illuminated green whenever the MS detector is On (that is, high voltage is supplied to the API source, mass analyzer, and ion detection system).

The LED labeled *Scanning* flashes blue whenever the MS detector is On and scanning ions.

Figure 2-4. Front panel LEDs of the MS detector

Two additional LEDs and a push-button switch are located on the front panel above the divert/inject valve. See Figure 2-5. When the divert/inject valve is set up for loop injections, the divert/inject valve button toggles the valve between load and inject modes and the labels *Load* and *Inject* apply. When the divert/inject valve is set up for divert valve operation, the divert/inject valve button toggles the LC flow between the MS detector and the waste container and the labels *Detector* and *Waste* apply.

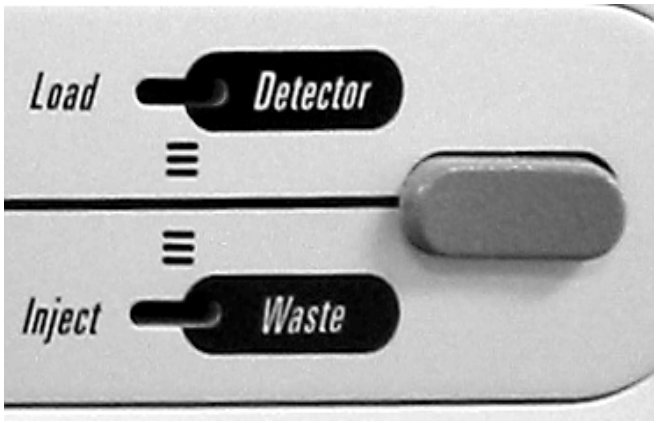


Figure 2-5. Divert/inject valve button and LEDs

The ***main power circuit breaker switch*** (labeled *Main Power*) is located on the power panel, which is located at the lower right corner of the right side panel of the MS detector. See Figure 2-6. In the Off (O) position, the circuit breaker removes all power to the MS detector, including the vacuum pumps. In the On (|) position, power is supplied to the MS detector. In the standard operational mode, the circuit breaker is kept in the On (|) position.

The ***electronics service switch*** is located on the power panel (See Figure 2-6). In the Service position the switch removes power to all components of the MS detector other than the vacuum system. In the Electronics Normal position power is supplied to all components of the MS detector.

> **Note.** To shut off all power to the MS detector in an emergency, place the main power circuit breaker switch (labeled *Main Power*) in the Off (O) position. Do not use the electronics service switch .

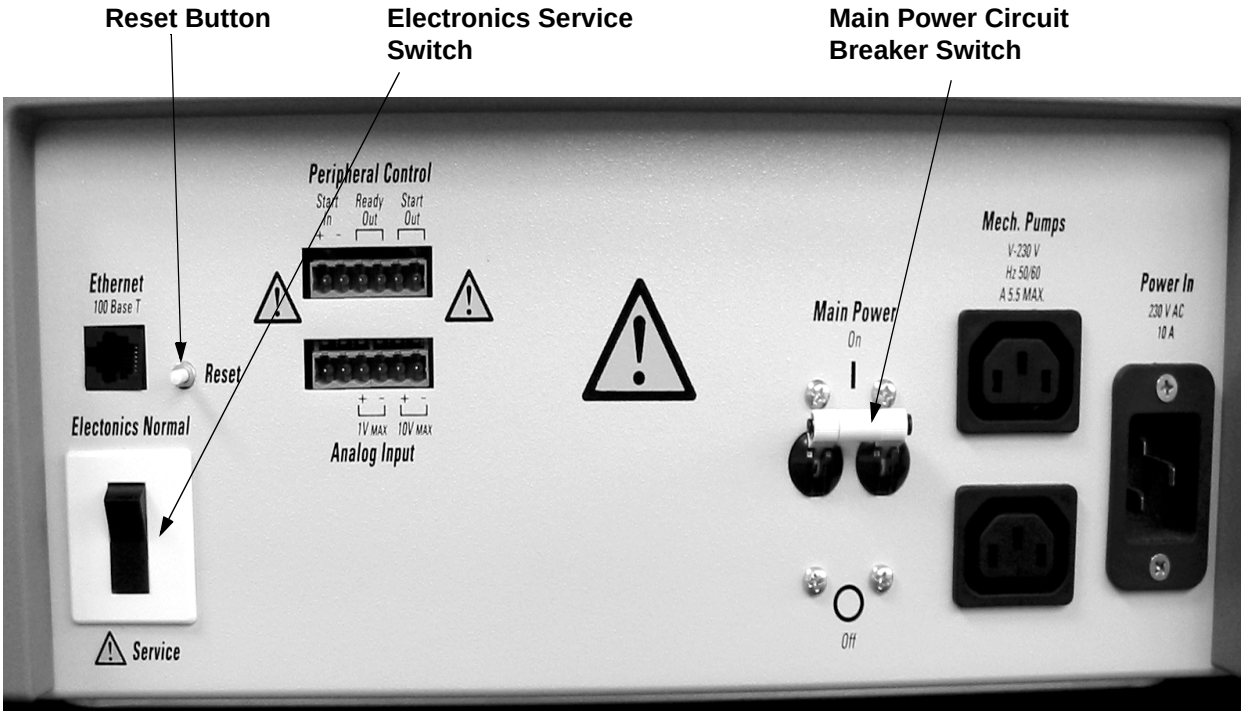


Figure 2-6. Power panel

The ***reset button*** (labeled *Reset*) is also located on the power panel. When you press the reset button for longer than 3 s, LTQ software is reloaded from the data system. Refer to the topic **Resetting the MS Detector** in the **System Shutdown, Startup, and Reset** chapter for information on resetting the MS detector.

API Source

The ***atmospheric pressure ionization (API) source*** forms gas phase sample ions from sample molecules that are contained in solution. The API source also serves as the interface between the LC and the MS detector. You can operate the API source using either the electrospray ionization (ESI), atmospheric pressure chemical ionization (APCI), atmospheric pressure photoionization (APPI), or nanospray ionization (NSI) technique.

The API source consists of:

- Ion Max™ ion source
- Ion source interface

Ion Max Ion Source

The Ion Max ion source is the part of the API source that is at atmospheric pressure. The Ion Max ion source can be configured to operate in any of several API modes, including: electrospray ionization (ESI), atmospheric pressure chemical ionization (APCI), nanospray ionization (NSI), and atmospheric pressure photoionization (APPI). See Figure 2-7. The ions produced in the API source are transmitted by the ion optics into the mass analyzer, where they are separated according to their mass-to-charge ratio.

Figure 2-7. Ion Max ion source with ESI probe attached

The Ion Max ion source housing allows you to quickly switch between ionization modes without the need for specialized tools. The ventilation of the ion source housing ensures that the housing is always cool and easy to handle. Pressure in the ion source housing is kept at atmospheric levels, which reduces the chemical noise that can be caused by nebulized gases when they are not properly evacuated from the ion source. The probe mounting angle is fixed at the optimum angle for signal intensity and ion source robustness. Minor adjustment of the probe position in the X, Y, and Z dimensions is allowed, with marked adjustments to allow for freedom in probe position

during ionization optimization. View ports are placed at the front and side of the ion source housing, which allows visual aid in positioning the probe during ESI operation, and enables easy addition of accessories.

Ion source lifetime is excellent due to several special features. The drain size and angle prevents ion source corrosion by allowing eluants to flow directly from the probe into the drain when auxiliary gases are off. For liquids that do not enter the drain directly, the floor of the ion source interior is specially sloped to enable maximum drainage of collected eluants. Additionally, the zero dead volume LC grounding union that connects the LC flow to the ESI sample inlet is offset from the ion source to prevent LC leaks from dripping directly on the ion source housing.

The Ion Max ion source incorporates a universal mounting platform and interface for use with ESI, APCI, NSI, and APPI ionization sources. For more information on the analysis of ions produced by the Ion Max ion source, please refer to **Finnigan Ion Max API Source Manual**.

Ion Source Interface

The ***ion source interface*** consists of the components of the API source that are held under vacuum (except for the atmospheric pressure side of the ion sweep cone). The ion source interface includes an ion transfer capillary, two cartridge heaters, heater block, platinum probe sensor, vent prevent ball, ion sweep cone, tube lens, and skimmer. See Figure 2-8 and Figure 2-9.

The ***ion transfer capillary*** assists in desolvating ions that are produced by ESI, APCI, NSI, or APPI. The capillary is an elongated, 2.5-in. cylindrical tube made of metal that has a hole bored through the center of its long axis. Two ***heater cartridges*** are embedded in the heater block. The ***heater block*** surrounds the ion transfer capillary and heats it to temperatures up to 400 °C. A ***platinum probe sensor*** measures the temperature of the heater block. Typical temperatures of the ion transfer capillary are 270 °C for ESI and 250 °C for APCI. Ions are drawn into the ion transfer capillary in the atmospheric pressure region and transported to the capillary-skimmer region of the vacuum manifold by a decreasing pressure gradient. A potential of typically 0 to ±10 V (positive for positive ions and negative for negative ions) assists in repelling ions from the ion transfer capillary to the skimmer. The ***vent prevent ball*** falls into the space occupied by the ion transfer capillary when the capillary is removed, thus preventing air from entering the vacuum manifold. The vent prevent ball allows you to remove the ion transfer capillary for cleaning without venting the system.

The ***ion sweep cone*** is a metallic cone over the capillary. The ion sweep cone acts as a physical barrier that protects the entrance of the capillary.

The system electronics include a voltage monitor circuit and an overtemperature/undertemperature circuit to protect the heaters. The voltage monitoring circuit detects shorting failures. The overtemperature portion of the circuit is intended to function as a thermal limit switch to prevent the

heater from turning on continuously above a preset temperature. The undertemperature feature identifies faults in the platinum probe sensor that would otherwise cause the heater to turn full on.

Ions from the ion transfer capillary enter the ***tube lens***. The tube lens has a mass dependent potential applied to it to focus the ions towards the opening of the skimmer. When you tune the LTQ, you adjust the tube lens offset voltage to maximize sensitivity by balancing desolvation with fragmentation.

Ions from the tube lens pass through the skimmer and move toward the Q00 quadrupole. The ***skimmer*** acts as a vacuum baffle between the higher pressure ion source interface region (at 1 Torr) and the lower pressure Q00 ion guide region (at 50 mTorr) of the vacuum manifold.

The ion source interface is enclosed in a vacuum chamber that is evacuated by the rotary-vane pump to a pressure of approximately 1 Torr.

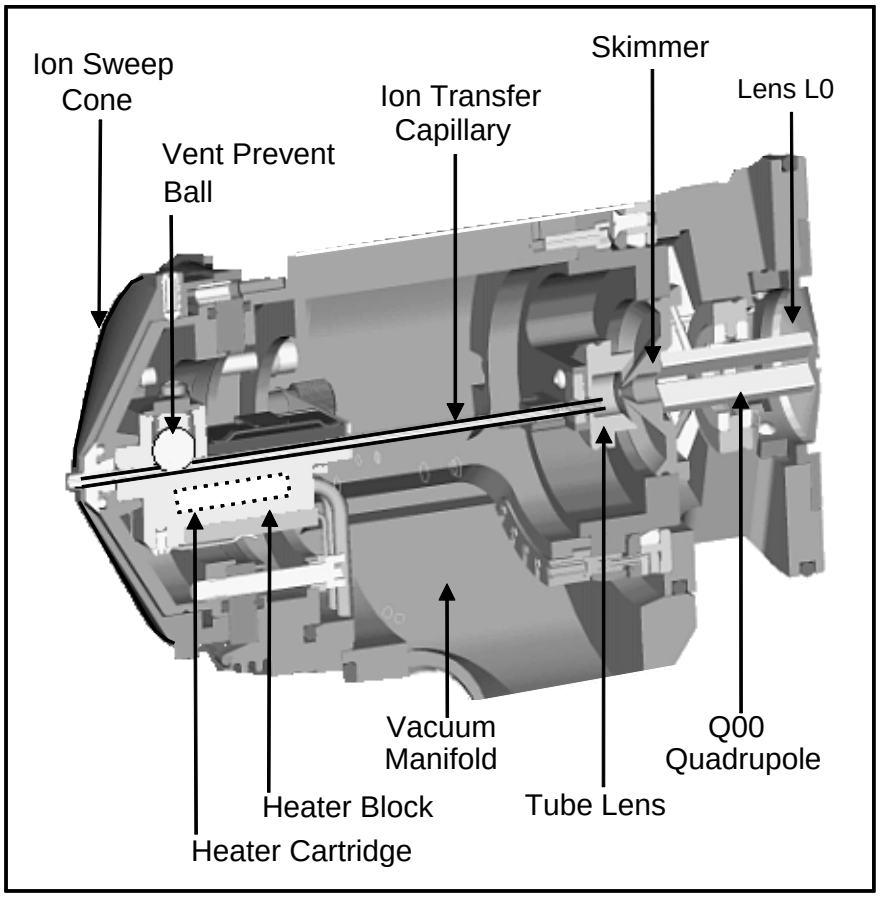


Figure 2-8. Cross sectional view of the ion source interface and Q00 ion guide

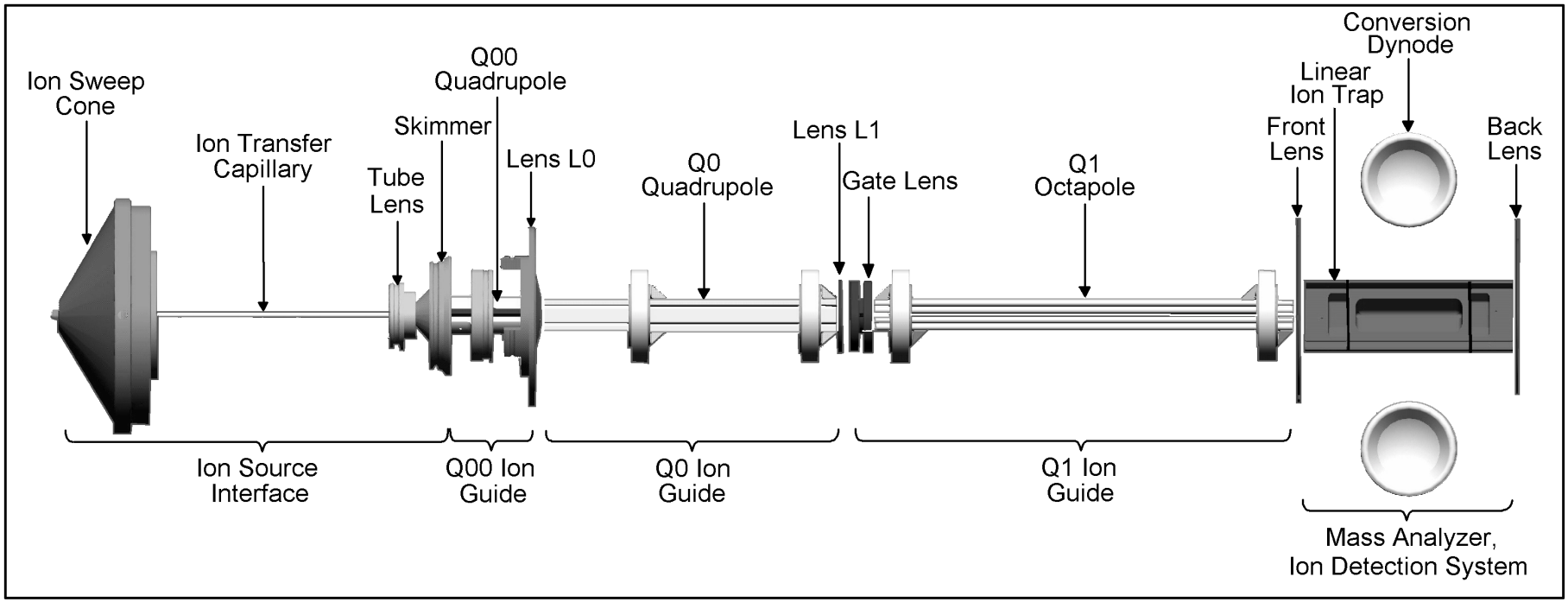


Figure 2-9. Internal (under vacuum) components of the MS detector

Ion Optics

The ***ion optics*** focus the ions produced in the API source and transmit them to the mass analyzer. The ion optics consist of three ion guides:

- Q00 ion guide
- Q0 ion guide
- Q1 ion guide

Q00 Ion Guide

The ***Q00 ion guide*** is the ion guide that is located closest to the API source. The Q00 ion guide includes the Q00 quadrupole and lens L0. See Figure 2-8 and Figure 2-9.

The ***Q00 quadrupole*** is a square array of square-profile rods that acts as an ion transmission device. An RF voltage that is applied to the rods gives rise to an electric field that guides the ions along the axis of the quadrupole. A dc voltage offset from ground applied to Q00—called the ***Q00 offset voltage***—increases the translational kinetic energy of ions emerging from the skimmer. During ion transmission, the offset voltage is negative for positive ions and positive for negative ions. Increasing the offset voltage will increase the translational kinetic energy of the ions. Typical values of the Q00 offset voltage are –4 V to +4 V.

The ***lens L0*** is a metal cylinder with a small hole in one end through which the ion beam can pass. A potential of between 0 and ±5 V (negative for positive ions and positive for negative ions) is applied to lens L0 to aid in ion transmission. Lens L0 also acts as a vacuum baffle between the Q00 and Q0 ion gauge chambers. The Q00 ion guide chamber of the vacuum manifold is evacuated to a pressure of 50 mTorr by the third inlet in the molecular drag section of the turbomolecular pump.

Q0 Ion Guide

The ***Q0 ion guide*** transmits ions from the Q00 ion guide to the Q1 ion guide. The Q0 ion guide includes the Q0 quadrupole and lens L1. See Figure 2-9.

The ***Q0 quadrupole*** is a square array of square-profile rods that acts as an ion transmission device similar to Q00. An RF voltage that is applied to the rods gives rise to an electric field that guides the ions along the axis of the quadrupole. The ***Q0 offset voltage*** increases the translational kinetic energy of ions emerging from Q00. Q0 must be at a lower potential than Q00. Because the gas pressure in Q00 is so high, ions typically have zero kinetic energy when they emerge from Q00. There must be a downhill potential gradient for them to enter Q0.

The ***lens L1*** is a metal disk with a circular hole in the center through which the ion beam can pass. An electrical potential can be applied to the lens to accelerate (or decelerate) ions as they approach the lens and to focus the ion beam as it passes through the lens. The value ranges between 0 and ±300 V. Lens L1 also acts as a vacuum baffle between the Q0 ion guide chamber and the mass analyzer chamber. The Q0 ion guide chamber is evacuated to a pressure of about 1 mTorr by the interstage inlet of the turbomolecular pump.

Q1 Ion Guide

The ***Q1 ion guide*** transmits ions from the Q0 ion guide to the mass analyzer. The Q1 ion guide includes the Q1 octapole and the gate lens. See Figure 2-9.

The ***Q1 octapole*** is an octagonal array of round-profile rods that acts as an ion transmission device similar to Q00 and Q0. An RF voltage that is applied to the rods gives rise to an electric field that guides the ions along the axis of the octapole. The ***Q1 offset voltage*** increases the translational kinetic energy of ions emerging from Q0.

The ***gate lens*** is used to start and stop the injection of ions into the mass analyzer.

Mass Analyzer

The ***mass analyzer*** is the site of mass analysis (that is, ion storage, ion isolation, collision induced dissociation, and ion scan out). This section describes the components of the mass analyzer, the voltages applied to the mass analyzer electrodes, the presence of helium damping gas in the mass analyzer cavity, and the operation of the mass analyzer during mass analysis.

Components of the Mass Analyzer

The mass analyzer consists of a front lens, linear ion trap, and back lens (Figure 2-9). The ***front*** and ***back lenses*** are metal disks with a circular hole in the center through which the ion beam can pass. An electrical potential of -21 V is applied to the front lens, and an electrical potential of +22 V is applied to the back lens. The purpose of the front and back lenses is to provide conductance limits. To clear ions from the trap, the ions are ejected through the back lens.

The basic design of the linear ion trap is shown in Figure 2-10. The ***linear ion trap*** is a square array of precision-machined and precision-aligned hyperbolic rods. Each rod is cut into three sections of 12, 37, and 12 mm length. Two of the center section rods, called the ***exit rods***, have a 0.25 x 30 mm slot through which the ions are ejected during scan out. Quartz spacers act as electrical insulators between adjacent rods. In each quadrupole rod section, rods opposite each other in the array are connected electrically. Thus, the four rods of each section can be considered to be two pairs of two rods each.

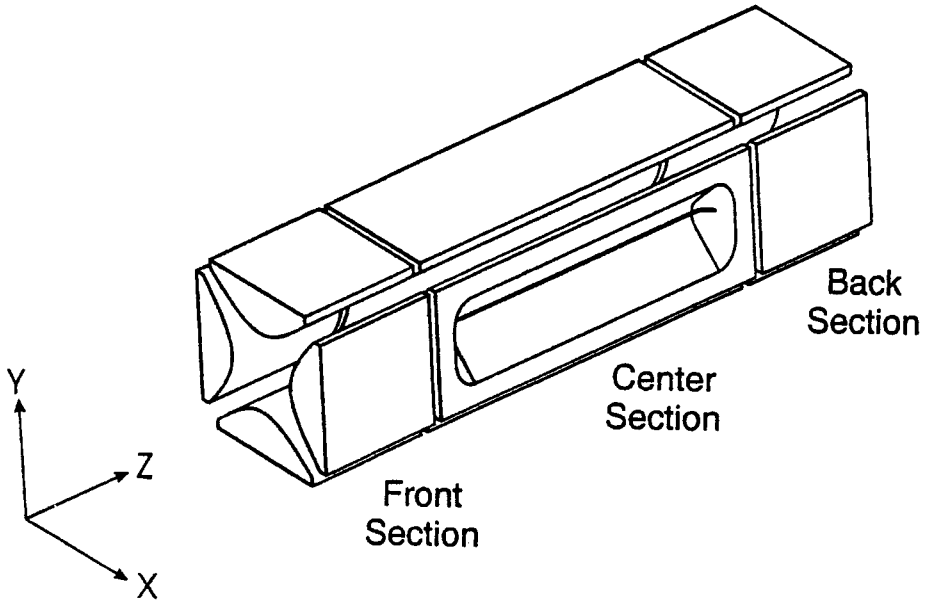


Figure 2-10. Linear ion trap quadrupome rod assembly

DC Axial Trapping Voltages

The LTQ uses three ***dc axial trapping voltages***, one for each rod section, which establish axial (Z-axis) trapping by lowering the potential of the center section below the potential of the front and back sections. For positively charged ions, LTQ applies a potential of -9 V to the front rod section during ion storage and a potential of +20 V during mass analysis. LTQ applies a potential of -12 V to the rear rod section during ion storage and a potential of +20 V during mass analysis. LTQ applies a potential of -14 V to the center rod section during both ion storage and mass analysis. For negatively charged ions the polarity of the dc axial trapping voltages are reversed.

Main RF Voltage

In each quadrupole rod section, rods opposite each other in the array are connected electrically. Ac voltages are applied to the rods and these voltages are ramped during the scan. Voltages of the same amplitude and sign are applied to the rods of each pair. However, the voltages applied to the different rod pairs are equal in amplitude but opposite in sign.

The ac voltage applied to the quadrupole rods is of constant frequency (1.2 MHz) and of variable amplitude (0 to 10,000 V peak-to-peak). Because the frequency of this ac voltage is in the radio frequency (RF) range, it is referred to as the ***main RF voltage***. The application of the main RF voltage to

the rod pairs produces a two-dimensional quadrupole field within the mass analyzer cavity. This time-varying field drives ionic motion in the radial (X,Y) direction. Ionic motion must be stable in the radial direction for an ion to remain trapped. (A stable trajectory is an oscillatory trajectory that is confined within the mass analyzer.) During ion scan out, the system produces a mass-dependent instability to eject ions from the mass analyzer in the radial direction.

When the amplitude of the main RF voltage is low, all ions above a minimum mass-to-charge ratio are trapped. This RF voltage is referred to as the ***storage voltage***, and the minimum mass-to-charge ratio is usually chosen to be greater than the mass-to-charge ratios associated with air, water, and solvent ions. During ion scan out, the main RF voltage is ramped at a constant rate corresponding to approximately 11,000 u/s (for unit resolution). As the main RF voltage increases, ions of increasing mass-to-charge ratio become successively unstable in the radial direction and are ejected from the mass analyzer. The voltage at which an ion is ejected from the mass analyzer is defined as its ***resonance voltage***. The ejection of ions of each mass-to-charge ratio occurs over a very short time. Many of these ions are detected by the ion detection system.

Ion Isolation Waveform Voltage, Resonance Excitation RF Voltage, and Resonance Ejection RF Voltage Applied to the Exit Rods

The ion isolation waveform voltage, resonance excitation RF voltage, and resonance ejection RF voltage are ac voltages that are applied to the exit rods to stimulate motion of the ions in the direction of the ion detection system. The voltages applied to the exit rods are equal in amplitude but are 180^{o} out of phase to one another. When the RF frequency applied to the rods equals the resonance frequency of a trapped ion, which depends on its mass, the ion gains kinetic energy. If the magnitude of the applied voltage is large enough or the ion is given sufficient time, the ion is ejected from the mass analyzer in the direction of the ion detection system (X direction).

The ***ion isolation waveform voltage*** consists of a distribution of frequencies between 5 and 500 kHz containing all resonance frequencies except for those corresponding to the ions to be trapped. The ion isolation waveform voltage acts during the ion isolation step of SIM, SRM, CRM, or MS^n ($n > 1$) full scan applications. The ion isolation waveform voltage, in combination with the main RF voltage, ejects all ions except those of a selected mass-to-charge ratio or narrow ranges of mass-to-charge ratios. The ion isolation waveform voltage is calculated by the LTQ and automatically applied at the correct time.

During the collision induced dissociation step of SRM, CRM, or MS^n ($n > 1$) full scan applications, the ***resonance excitation RF voltage*** is applied to the exit rods to fragment parent ions into product ions. The resonance excitation RF voltage is not strong enough to eject an ion from the mass analyzer.

However, ion motion in the radial direction is enhanced and the ion gains kinetic energy. After many collisions with the helium damping gas, which is present in the mass analyzer, the ion gains enough internal energy to cause it to dissociate into product ions. The product ions are then mass analyzed.

During ion scan out, the ***resonance ejection RF voltage*** facilitates the ejection of ions from the mass analyzer and thus improves mass resolution. The resonance ejection RF voltage is applied at a fixed frequency and increasing amplitude during the ramp of the main RF voltage. Only when an ion is about to be ejected from the mass analyzer cavity by the main RF voltage is it in resonance with the resonance ejection RF voltage. When an ion approaches resonance, it moves farther away from the center of the mass analyzer, where the field generated by the main RF voltage is zero (and space-charge effects are strong), into a region where the field produced by the main RF voltage is strong (and space-charge effects are small). As a result, the ejection of the ion is facilitated, and mass resolution is significantly improved.

Helium Damping Gas in the Mass Analyzer Cavity

The mass analyzer cavity contains helium that is used as a damping gas and a collision activation partner. The helium damping gas enters the mass analyzer cavity through a gap between the quadrupole rods. The flow of gas (~1 mL/min) into the mass analyzer cavity is regulated by a pressure regulator and a capillary restrictor. The flow of gas out of the mass analyzer cavity (and into the turbomolecular pump) is restricted by the openings in the mass analyzer. The flows into and out of the cavity are matched so that the partial pressure of helium in the mass analyzer cavity is maintained at approximately 0.1 Pa (10^{-3} Torr).

The collisions of the ions entering the mass analyzer with the helium slow the ions so that they can be trapped by the RF field in the mass analyzer.

The presence of helium in the mass analyzer cavity significantly enhances sensitivity and mass spectral resolution. Before their ejection from the mass analyzer cavity, sample ions collide with helium atoms. These collisions reduce the kinetic energy of the ions, thereby damping the amplitude of their oscillations. As a result, the ions are focused to the axis of the cavity rather than being allowed to spread throughout the cavity.

Helium in the mass analyzer cavity also serves as a collision activation partner. During the collision induced dissociation step of an SRM, CRM, or MS^n ($n > 1$) full scan analysis, the resonance excitation RF voltage applied to the endcap electrodes drives parent ions into the helium atoms. After gaining sufficient internal energy from the resulting collisions, the parent ion dissociates into one or more product ions.

Summary of Mass Analyzer Operation

The processes that occur in the mass analyzer can be broken down into four steps:

- Ion storage
- Ion isolation (SIM, SRM, CRM, or MS^n (n > 1) full scan only)
- Collision induced dissociation (SRM, CRM, or MS^n (n > 1) full scan only)
- Ion scan out (the ion detection step)

For SRM and MS/MS full scan applications the ion isolation and collision induced dissociation steps are performed once. For CRM and MS^n (n > 1) full scan applications the ion isolation and collision induced dissociation steps are performed n-1 times.

Before ion storage, the following conditions are established:

- Helium is present in the mass analyzer cavity at a partial pressure of about 0.1 Pa (10^{-3} Torr).
- Main RF voltage is set to the storage voltage.
- Dc axial trapping voltages are set to the storage voltages.
- Ion isolation waveform voltage, resonance excitation RF voltage, and resonance ejection RF voltage on the exit rods are off.

With these conditions achieved, sample ions formed in the API source are trapped in the mass analyzer if the ions have mass-to-charge ratios greater than the minimum storage mass-to-charge ratio.

Next, for SIM, SRM, CRM, or MS^n (n > 1) full scan, the ion isolation waveform voltage is applied to the exit rods, in combination with a ramp of the main RF voltage to a new storage voltage, to eject all ions except those of the selected mass-to-charge ratio.

Then, for SRM, CRM, or MS^n (n > 1) full scan analyses, the resonance excitation RF voltage is applied to the exit rods to cause collision induced dissociation. Product ions with mass-to-charge ratio greater than the minimum storage mass-to-charge ratio are stored. (The minimum storage mass during collision induced dissociation is typically set to one quarter of the parent ion mass-to-charge ratio.)

For SRM and MS/MS full scan applications the ion isolation and collision induced dissociation steps are performed once. For CRM and MS^n (n > 1) full scan applications the ion isolation and collision induced dissociation steps are performed n-1 times.

Finally, the sample ions or product ions are scanned out: The main RF voltage is ramped from low voltage to high voltage, and simultaneously the resonance ejection RF voltage is applied to the exit rods to facilitate ejection. As the main RF voltage is increased, ions of greater and greater mass-to-charge

ratios become unstable and are ejected through the slots in the exit rods. Many of these ions are focused toward the ion detection system where they are detected.

Ion Detection Systems

The LTQ is equipped with a two high sensitivity, off-axis ***ion detection systems*** that produce a high signal-to-noise ratio and allows for voltage polarity switching between positive ion and negative ion modes of operation. Each ion detection system includes a 15-kV conversion dynode and a channel electron multiplier. The ion detection systems are located on opposite sides of the mass analyzer. See Figure 2-11.

The ***conversion dynode*** is a concave metal surface that is located at a right angle to the ion beam. A potential of +15 kV for negative ion detection or -15 kV for positive ion detection is applied to the conversion dynode. When an ion strikes the surface of the conversion dynode, one or more secondary particles are produced. These secondary particles can include positive ions, negative ions, electrons, and neutrals. When positive ions strike a negatively charged conversion dynode, the secondary particles of interest are negative ions and electrons. When negative ions strike a positively charged conversion dynode, the secondary particles of interest are positive ions. These secondary particles are focused by the curved surface of the conversion dynode and are accelerated by a voltage gradient into the electron multiplier. The ***conversion dynode shield***, ***tube***, and ***disk*** shield the vacuum manifold from the electric field produced by the conversion dynode.

The electron multiplier is mounted on the top cover plate of the vacuum manifold next to the mass analyzer. See Figure 2-11 and Figure 2-16. The ***electron multiplier*** includes a cathode and an anode. The ***cathode*** of the electron multiplier is a lead-oxide, funnel-like resistor. A potential of up to -2.5 kV is applied to the cathode by the ***high voltage ring***. The exit end of the cathode (at the anode) is near ground potential. The cathode is held in place by the high voltage ring, two ***support plates***, the ***electron multiplier support***, and the ***electron multiplier shield***. A spring washer applies a force to the cathode to hold it in contact with the electron multiplier shield. The electron multiplier support is attached to the top cover plate of the vacuum manifold by two screws.

The ***anode*** of the electron multiplier is a small cup located at the exit end of the cathode. The anode collects the electrons produced by the cathode. The anode screws into the anode feedthrough in the top cover plate.

Secondary particles from the conversion dynode strike the inner walls of the electron multiplier cathode with sufficient energy to eject electrons. The ejected electrons are accelerated farther into the cathode, drawn by the increasingly positive potential gradient. Due to the funnel shape of the cathode, the ejected electrons do not travel far before they again strike the inner surface of the cathode, thereby causing the emission of more electrons.

Thus, a cascade of electrons is created that finally results in a measurable current at the end of the cathode where the electrons are collected by the anode. The current collected by the anode is proportional to the number of secondary particles striking the cathode.

Typically, the electron multiplier is set to a gain of about 3×10^5 (i.e., for each ion or electron that enters, 3×10^5 electrons exit). The current that leaves the electron multiplier via the anode is converted to a voltage by the electrometer circuit and recorded by the data system. Refer to the topic **Ion Detection System Electronic Assemblies** on page 2-38.

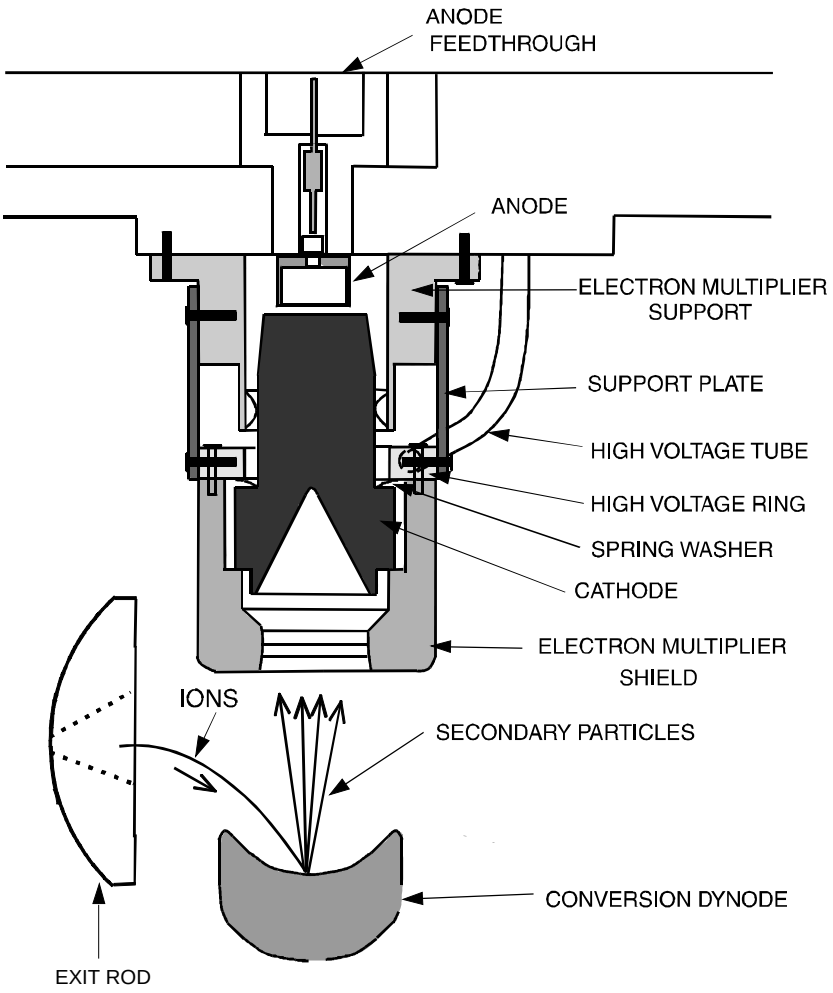


Figure 2-11. Cross sectional view of the ion detection system, showing the electron multiplier and the conversion dynode

The ion detection system of the LTQ increases signal and decreases noise. The high voltage applied to the conversion dynode results in a high conversion efficiency and increased signal. That is, for each ion striking the conversion dynode, many secondary particles are produced. The increase in conversion efficiency is more pronounced for more massive ions than for less massive ions.

Because of the off-axis orientation of the ion detection system relative to the mass analyzer, neutral molecules from the mass analyzer tend not to strike the conversion dynode or electron multiplier. As a result, the noise from neutral molecules is reduced.

Vacuum System and Inlet Gasses Hardware

The ***vacuum system*** evacuates the region around the API stack, ion optics, mass analyzer, and ion detection system. The principal components of the vacuum system include the following (see Figure 2-12):

- Vacuum manifold
- Turbomolecular pump
- Forepump
- Convectron® gauge
- Ion gauge

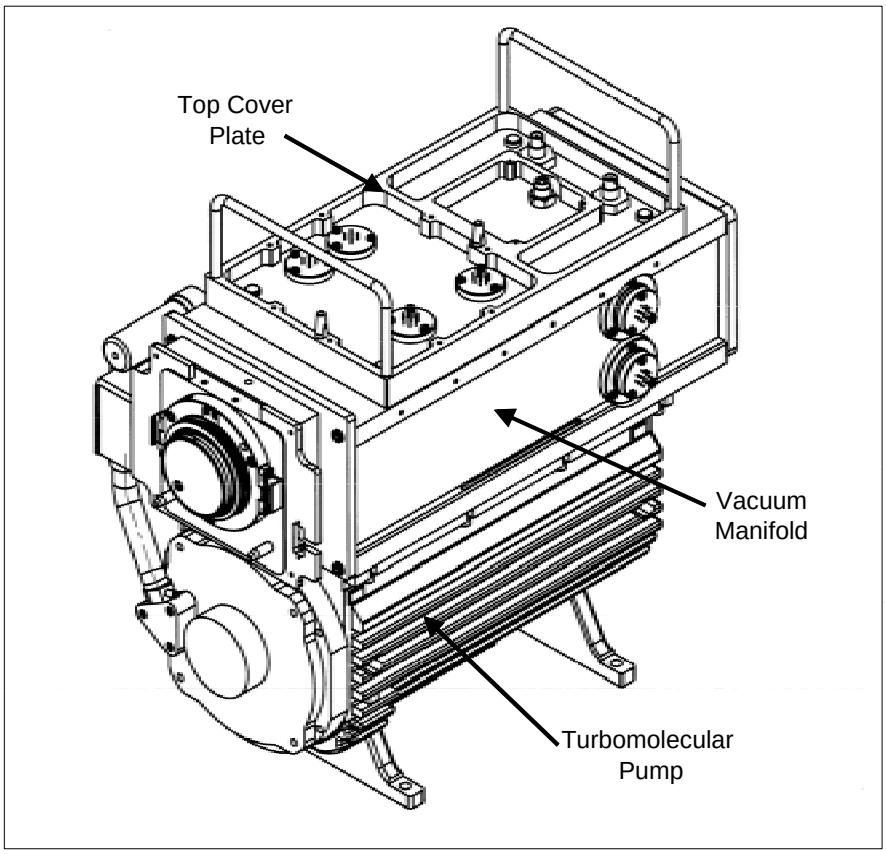


Figure 2-12. Vacuum manifold with top cover plate and turbomolecular pump

The ***inlet gasses hardware*** controls the flow of damping gas, sheath gas, auxiliary gas, sweep gas, and air (during venting) into the MS detector. The inlet gasses hardware includes the following components:

- Vent gas valve
- Damping gas inlet assembly
- Sheath gas valve
- Auxiliary gas valve
- Sweep gas valve

A functional block diagram of the vacuum system and inlet gasses hardware is shown in Figure 2-13.

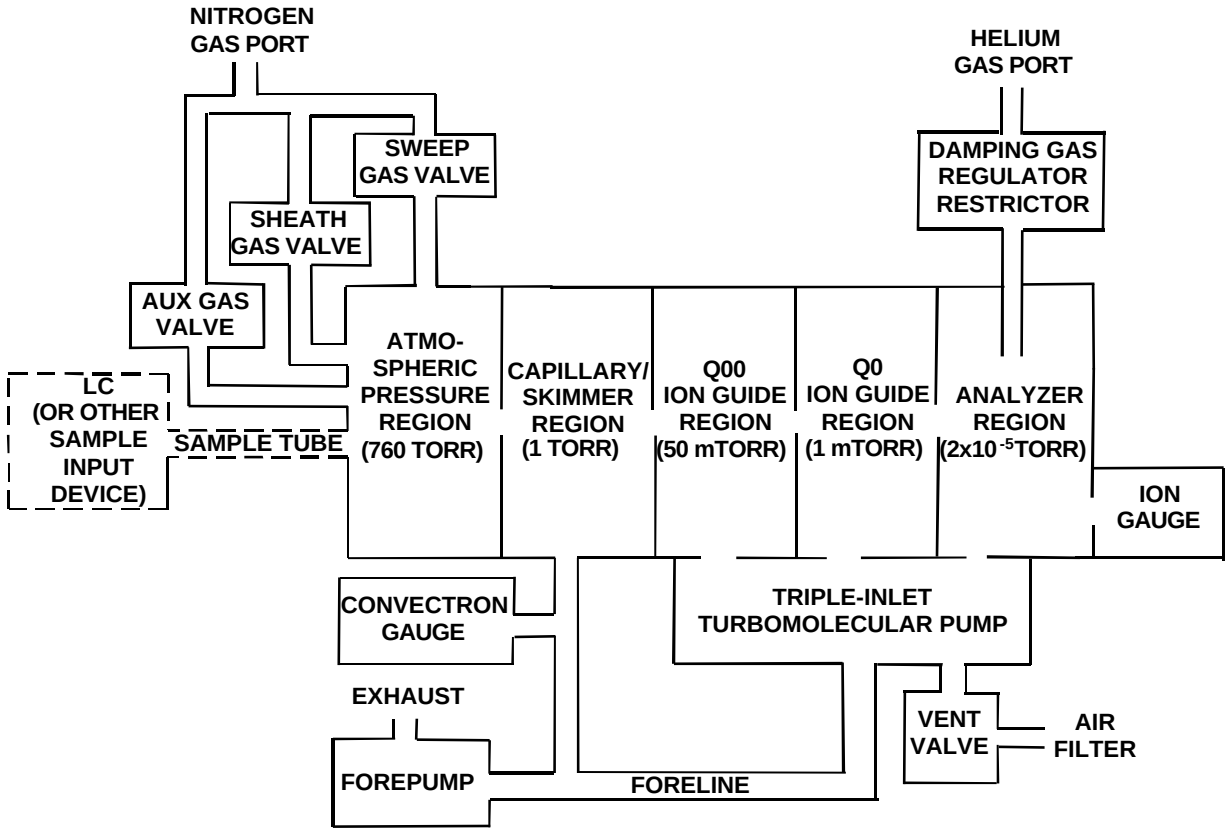


Figure 2-13. Functional block diagram of the vacuum system and inlet gasses hardware

Vacuum Manifold

The ***vacuum manifold*** encloses the ion source interface, ion guides, mass analyzer, and ion detection system assemblies. The vacuum manifold is a thick-walled, aluminum chamber with a removable top cover plate, machined flanges on the front, sides, and bottom, and various electrical feedthroughs and gas inlets.

The vacuum manifold is divided into four chambers by three baffles. See Figure 2-14. The region inside the first chamber, called the ***capillary/skimmer region***, is evacuated to 1 Torr by the rotary-vane pump. The region inside the second chamber, called the ***Q00 ion guide region***, is evacuated to 50 mTorr by the third inlet in the molecular drag section of the triple-inlet turbomolecular vacuum pump. The region inside the third chamber, called the ***Q0 ion guide region***, is evacuated to 1 mTorr by the interstage port of the turbomolecular vacuum pump. The region inside the fourth chamber, called the ***analyzer region***, is evacuated to less than 10^{-5} Torr by the high vacuum port of the turbomolecular pump. The turbomolecular pump in turn discharges into the rotary-vane pump through the foreline.

Three high-voltage electrical feedthroughs pass through the vacuum manifold:

- Two feedthroughs for the high voltage for the conversion dynodes
- A feedthrough for the RF voltage and DC voltages of the mass analyzer

The vacuum manifold also has an opening for the ion gauge.

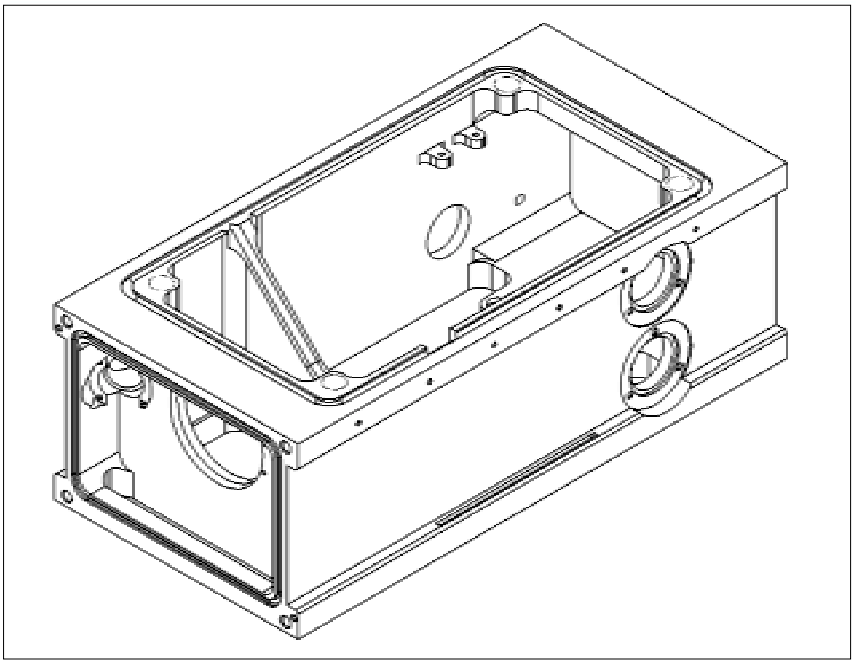


Figure 2-14. Vacuum manifold

The removable ***top cover plate*** of the vacuum manifold holds the Q0 and Q1 ion guides, mass analyzer, and two electron multipliers (one part of the ion detection system). Thus, removal of the top cover plate allows easy access to these assemblies. Two handles on the top and four guide posts on the underside of the top cover plate facilitate its removal and installation. An electrically conductive O-ring provides a vacuum-tight seal between the top cover plate and the vacuum manifold. The top cover plate and its attached assemblies are shown in Figure 2-15 and Figure 2-16.

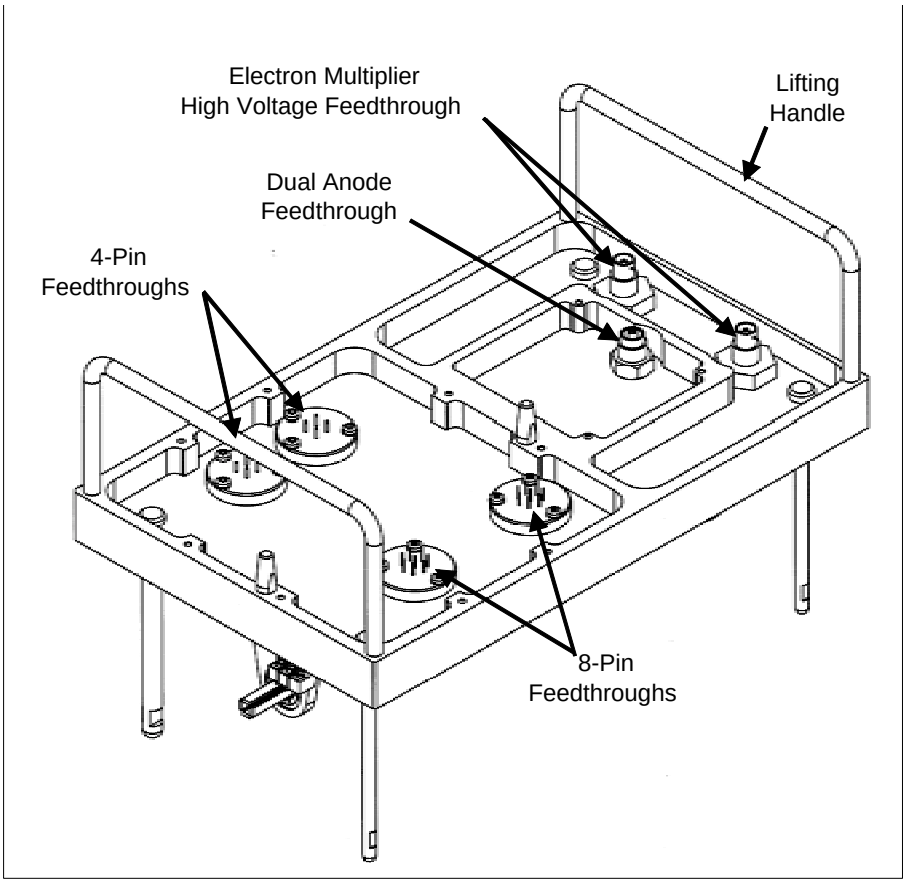


Figure 2-15. Top cover plate of the vacuum manifold (topside)

Seven electrical feedthroughs pass through the top cover plate:

- Two 4-pin and two 8-pin feedthroughs for the RF and DC voltages for the ion optics
- Two feedthroughs for the high voltage for the cathodes of the electron multipliers
- A feedthrough for the ion current signal from the dual anode of the electron multipliers

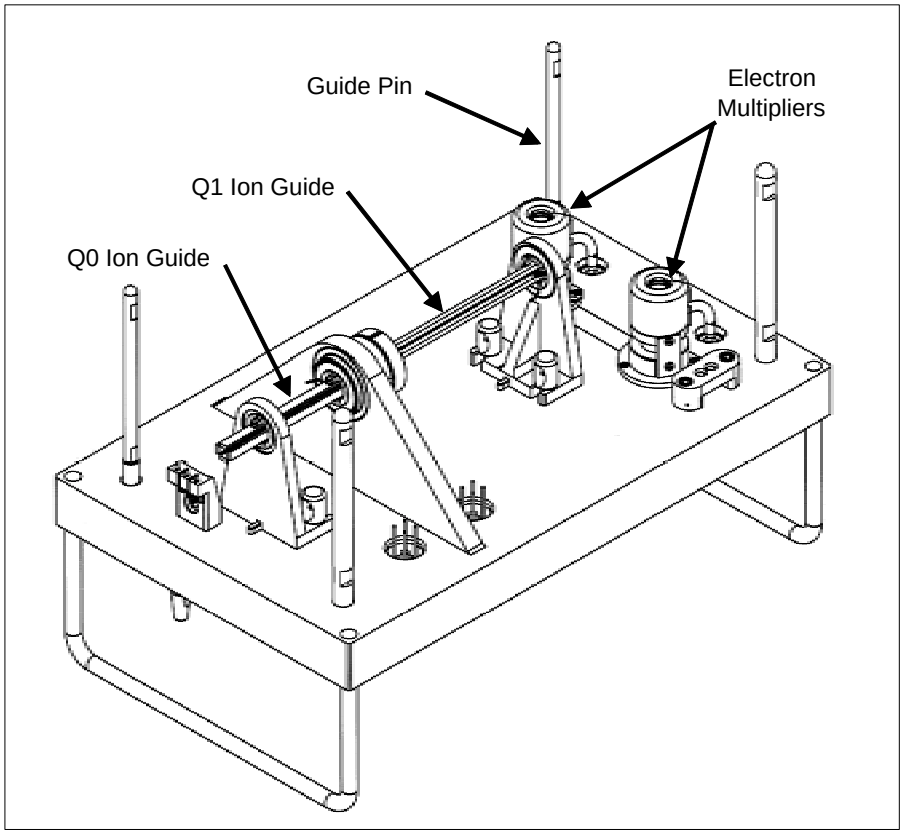


Figure 2-16. Top cover plate of the vacuum manifold (underside), and attached assemblies

Turbomolecular Pump

A Leybold TW220/150/15S triple-inlet ***turbomolecular pump*** provides the vacuum for the Q00 ion guide region, Q0 ion guide region, and analyzer region of the vacuum manifold. The turbomolecular pump mounts onto the bottom of the vacuum manifold.

The turbomolecular pump has three pumping inlets (see Figure 2-17):

- A 400 L/s high-vacuum inlet at the top of the rotor stack, which evacuates the analyzer chamber
- An 300 L/s interstage inlet about half way down the rotor stack, which evacuates the Q0 ion guide chamber
- A 25 L/s third inlet in the molecular drag section of the pump, which evacuates the Q00 ion guide chamber

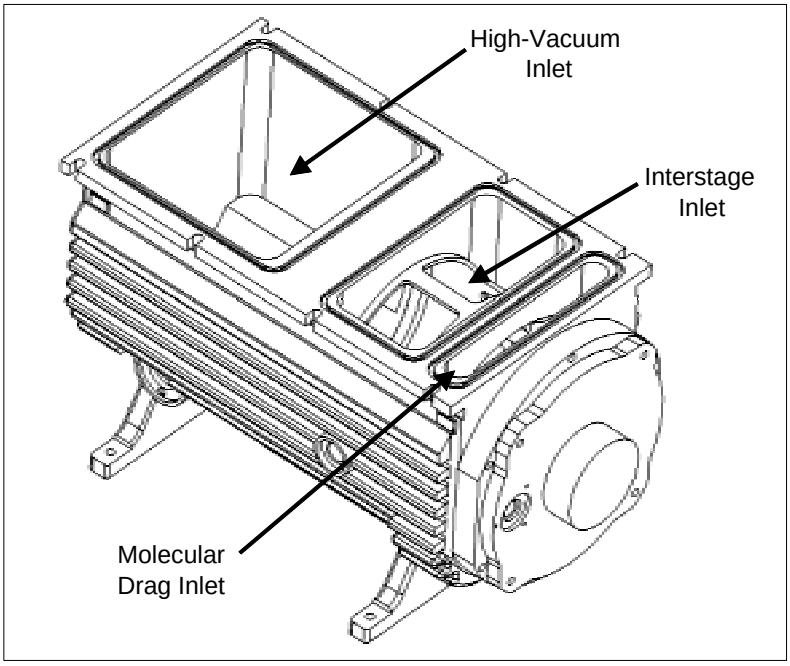


Figure 2-17. Turbomolecular pump

The turbomolecular pump is controlled by a Leybold TDS controller and powered by a +24 V dc (250 W) power supply. Power for the turbomolecular pump is turned off by the the main power circuit breaker switch, but not by the electronics service switch. The pump is air cooled by a fan that draws air in from the front of the instrument.

The Leybold TDS ***Turbomolecular Pump Controller*** provides power to and control of the turbomolecular pump. The turbomolecular pump status (temperature, rotational speed, etc.) is sent from the Turbomolecular Pump Controller to the embedded computer over a serial line. Power to the turbomolecular pump is shut off if the foreline pressure, as measured by the Convectron gauge, is too high, or if the turbomolecular temperature is too high.

Forepump

An Edwards E2M30 ***forepump*** (or mechanical pump) establishes the vacuum necessary for the proper operation of the turbomolecular pump. The forepump also evacuates the ion transfer capillary-skimmer region of the vacuum manifold. The pump has a maximum displacement of 650 L/min and maintains a minimum pressure of approximately 100 Pa (1 Torr).

The forepump is connected to the turbomolecular pump by a section of 3.8 cm (1.5 in.) ID reinforced PVC tubing. The power cord of the forepump is plugged into the outlet labeled *Mech. Pumps* on the power panel (See Figure 2-6 on page 2-10). This outlet supplies power to the pump and is controlled by the main power circuit breaker switch and not by the electronics service switch.

> **Caution.** Always plug the forepump power cord into the outlet labeled *Mech. Pumps* on the right side of the MS detector. Never plug it into a wall outlet.

Convectron Gauge

The ***Convectron gauge*** measures the pressure in the ion transfer capillary-skimmer region of the vacuum manifold and the foreline, which connects the turbomolecular pump and the forepump. The pressure measured by the Convectron gauge is monitored by the Signal/Power Distribution PCB. The Signal/Power Distribution PCB detects whether the foreline pressure is too high for the proper operation of the turbomolecular pump.

Ion Gauge

The pressure in the analyzer region of the vacuum manifold is measured by a Granville-Phillips® 342™ mini ion gauge. The ***ion gauge*** produces energetic electrons that cause the ionization of molecules in the ion gauge. Positive ions formed in the ion gauge are attracted to a collector. The collector current is related to the pressure in the vacuum manifold. The ion gauge is also involved in vacuum protection.

Vent Valve

The ***vent valve*** allows the vacuum manifold to be vented to air that has been filtered through a sintered nylon filter. The vent valve is a solenoid-operated valve. The vent valve is closed when the solenoid is energized.

The vacuum manifold is vented when external power is removed from the MS detector. (Power is removed from the MS detector by a power failure or by placing the main power circuit breaker in the Off (O) position.) Power is provided to the vent valve for 30 s after the external power is removed. If external power is not restored to the MS detector in 30 s, power to the vent valve solenoid is shut off. When power to the vent valve solenoid is shut off, the vent valve opens and the manifold is vented to filtered air. The vent valve closes after power is restored to the MS detector.

Damping Gas Inlet Assembly

The ***damping gas inlet assembly*** controls the flow of helium into the mass analyzer cavity. Helium (40 ±10 psig [275 ±70 kPa], 99.999% [ultra-high] purity) enters the MS detector through a 1/8-in. port on the rear of the MS detector. LTQ regulates the flow of helium by use of a capillary restrictor and a pressure regulator on the helium line. The helium enters the mass analyzer through a nipple on the exit endcap electrode.

Helium in the mass analyzer cavity dampens ionic motion and improves the performance of the MS detector. Refer to the topic **Helium Damping Gas in the Mass Analyzer Cavity** on page 2-19.

Sheath Gas, Auxiliary Gas, and Sweep Gas Valves

The ***sheath gas, auxiliary gas, and sweep gas valves*** control the flow of nitrogen into the API source. The ***sheath gas*** is the inner coaxial nitrogen gas of the API probe that sprays (nebulizes) the sample solution into a fine mist as it exits the sample tube. The ***auxiliary gas*** is the outer coaxial nitrogen gas that assists the sheath gas in the nebulization and evaporation of sample solutions. The ***Sweep gas*** flows out from behind the sweep cone in the ion source interface. Sweep gas aids in solvent declustering and adduct reduction.

Dry nitrogen (100 ±20 psig [690 ±140 kPa], 99% purity) enters the MS detector through a 1/4-in. port in the rear of the MS detector. The nitrogen pressure is regulated by valves that are controlled by the data system. You can set the flow rates from the Tune Plus window. Sheath gas is not used with an NSI source. The sheath gas, auxilary gas, and sweep gas enter the API source through 1/8-in. ID tubing.

Cooling Fans

Five fans provide cooling for the MS detector. One 21 $ft.^3$/min. fan cools the RF voltage coil. One 21 $ft.^3$/min. fan cools the turbomolecular pump. Three 100 $ft.^3$/min. fans cool the electronics in the tower. Air is drawn in from the rear of the MS detector. The exhaust air is expelled from the vent slots on the sides of the MS detector.

> **Caution**. To ensure proper cooling, the MS detector must always be operated with its covers in place.

Electronic Assemblies

The electronic assemblies that control the operation of the MS detector are distributed among various printed circuit boards (PCBs) and other modules located in the electronics rack and on or around the vacuum manifold of the MS detector.

The electronic assemblies of the MS detector include the following:

- Power Module and power distribution assemblies
- System control and monitoring circuitry
- RF/waveform voltage generation electronic assemblies
- Ion detection system electronic assemblies

Power Entry Module and Power Distribution

The ***Power Entry Module*** provides system power control, a contact closure interface, an Ethernet 100 Base T connection from the Power/Signal Distribution PCB to the data system PC, and a system reset button. See Figure 2-6 on page 2-10.

The Power Entry Module accepts line power, filters it, and provides it to various components of the MS detector. The Power Entry Module includes the following components:

- Main power circuit breaker switch
- Line filter
- Electronics service switch
- Interlock PCB

A functional block diagram of the Power Entry Module and MS detector power distribution is shown in Figure 2-18.

Line power (230 V ac ± 10%, 15 A, 50/60 Hz, single phase) enters the power panel on the right side panel of the MS detector, passes through the main power circuit breaker and then to a line filter (see Figure 2-6).

The ***main power circuit breaker switch***, located on the right side panel of the MS detector (see Figure 2-6), shuts off all power to the MS detector, including the vacuum system. After the main power circuit breaker switch, power goes to the line filter.

The ***line filter*** removes noise from the line power.

After the line filter, power goes to the Power/Signal Distribution PCB and to the electronics service switch.

The ***electronics service switch*** is a circuit breaker that allows service of the non-vacuum system components of the MS detector with the vacuum system still in operation (see Figure 2-6). In the Service position the switch removes

power to all components of the MS detector other than the fans and vacuum system. In the Electronics Normal position power is supplied to all components of the MS detector.

> **Note.** For emergency shutoff of all power to the MS detector, place the main power circuit breaker switch in the Off (O) position. Do not use the electronics service switch to remove power to the system in an emergency.

The ***Interlock PCB***, which resides in the Power Module, receives 220 V ac from after the electronics service switch (called *service 220 V ac*) and +24 V dc from PS2 power supply via the Power/Signal Distribution PCB. If the safety interlock switch on the API source is closed, then the Interlock PCB distributes 220 V ac to the APCI vaporizer heater and +24 V dc (called *interlock +24 V dc*) to the Power/Signal Distribution PCB, which distributes it to the 300 V power supply, 8 KV power supply, and the conversion dynode/electron multiplier power supply.

The ***Power/Signal Distribution PCB*** receives 220 V ac and service 220 V ac from the Power Module. The Power/Signal Distribution PCB distributes the 220 V ac to power supply PS2 and the service 220 V ac to power supply PS1. It then distributes the power produced by PS1 and PS2 to other power supplies, PCBs, turbomolecular pump, vent valve, and fans. The Power/Signal Distribution PCB also receives the interlock +24 V dc from the Interlock PCB and distributes it to the 300 V power supply, the 8 KV power supply, and the conversion dynode/electron multiplier power supply.

Power supply PS1 provides +5 V dc, ± 15 V dc for analog and digital circuits and +60 V dc for the heater that heats the ion transfer capillary.

Power supply PS2 provides +24 V dc for the turbomolecular pump, fans, vent valve, divert/inject valve, syringe pump, 8 KV power supply, conversion dynode/electron multiplier power supply, Main RF PCB, and Analog PCB. It also provides +36 V dc and -28 V dc that is used for RF generation for the ion guides and mass analyzer.

The ***300 V power supply*** provides the ± 300 V dc and ± 150 V dc that is used by the Analog PCB to produce lens and dc offset voltages for the ion source interface, ion optics, and mass analyzer.

The ***Source PCB*** distributes power to the ion gauge, divert/inject valve, syringe pump, and nitrogen and helium gas valves.

The ***8 kV power supply*** delivers voltage to either the ESI needle in the ESI mode, or the corona discharge needle in the APCI mode. Typical operating voltages range between ±3 to ±6 kV. In the ESI mode, the voltage is regulated, whereas in the APCI mode, the current is regulated.

The ***conversion dynode / electron multiplier power supply*** provides ±15 kV to the conversion dynodes and 0 to –2.5 KV to the electron multipliers in the ion detection system.

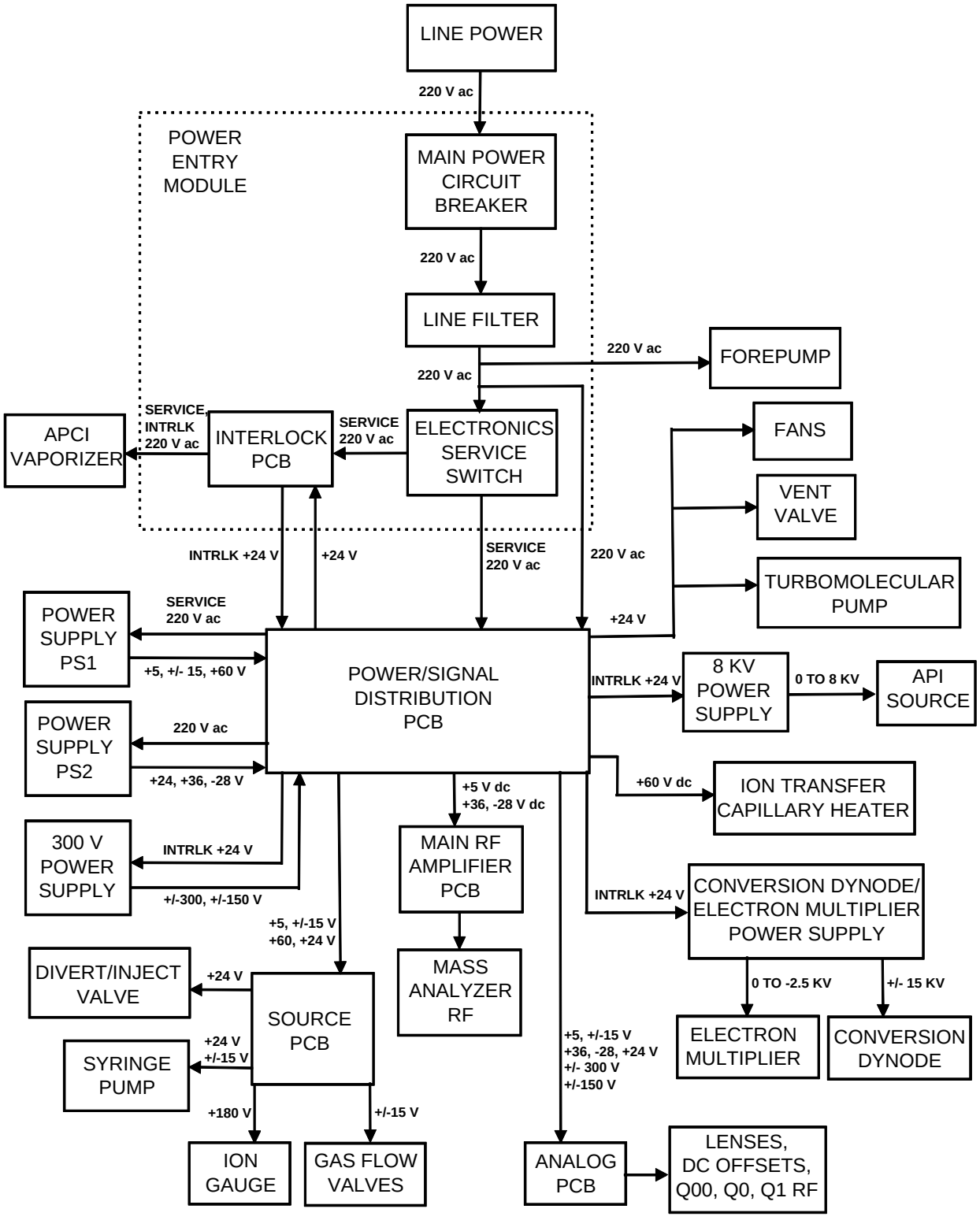


Figure 2-18. Functional block diagram of the Power Entry Module and power distribution of the MS detector

System Control and Monitoring Circuitry

The LTQ electronics contains the following circuits for controlling and monitoring the operation of the MS detector:

- Dc voltage control circuitry
- Divert/inject valve control circuit
- API source control circuit
- Electron multiplier control circuit
- Conversion dynode control circuit
- Ion transfer capillary heater/sensor control circuit
- APCI vaporizer heater/sensor control circuit/safety interlock relay
- Ion gauge control circuit
- Convectron® gauge control circuit
- Vacuum protection circuitry
- RF voltage control circuitry
- Temperature monitoring circuitry
- Diagnostic circuitry

The ***dc voltage control circuitry*** controls and monitors the dc voltages that are applied to the ion transfer capillary heater, tube lens, ion optics, lenses, and mass analyzer electrodes.

The ***divert/inject valve control circuit*** controls and monitors the divert/inject valve.

The ***API source control circuit*** controls and monitors the high voltage that is applied to the ESI needle, the APCI corona discharge needle, and the NSI capillary.

The ***electron multiplier control circuit*** sends a signal to the electron multiplier power supply that is proportional to the voltage to be applied to the electron multiplier cathode. It also reads back a signal that is proportional to the actual voltage applied to the electron multiplier cathode. The electron multiplier control circuit lowers the electron multiplier voltage when mass analysis is not occurring.

The ***conversion dynode control circuit*** controls and monitors the polarity of the 15 kV potential that is applied to the conversion dynode.

The ***ion transfer capillary heater/sensor control circuit*** monitors the temperature of the ion transfer capillary via a platinum probe temperature sensor. It also provides the voltage needed by the ion transfer capillary heater.

The ***APCI vaporizer heater/sensor control circuit*** controls the temperature of the APCI vaporizer via a thermocouple sensor. It also provides 230 V ac line voltage to the heater in the APCI vaporizer.

The ***ion gauge control circuit*** controls the ion gauge and reads back the pressure signal. (The ion gauge measures the pressure in the analyzer region of the vacuum manifold.)

The ***Convectron gauge control circuit*** controls the Convectron gauge and reads back the pressure signal. (The Convectron gauge measures the pressure in the foreline and the ion transfer capillary-skimmer region of the vacuum manifold.)

The ***vacuum protection circuitry*** monitors the pressure in the ion transfer capillary-skimmer region of the vacuum manifold, as measured by the Convectron gauge, and in the analyzer region of the vacuum manifold, as measured by the ion gauge. The vacuum protection circuitry turns off power to the ion optics and mass analyzer RF and waveform generation circuitry, 8 kV power supply (for the API source), electron multiplier and conversion dynode power supply, APCI vaporizer heater, and dc voltages to the ion transfer capillary heater, tube lens, ion optics, and mass analyzer if one or more of the following conditions arise:

- The pressure in the ion transfer capillary-skimmer region is above 3 Torr
- The pressure in the analyzer region is above 5×10^{-4} Torr
- The high-voltage safety interlock switch on the API source is open (that is, the door to the Ion Max ion source is open)

The LED labeled *Vacuum* on the front panel of the LTQ is illuminated green whenever the vacuum protection circuitry indicates that the vacuum is OK (and the safety interlock switch on the API source is closed).

The ***RF voltage control circuitry*** controls and monitors the PCBs that are responsible for RF voltage generation.

The ***temperature monitoring circuitry*** monitors the temperatures at several PCBs in the MS detector.

The ***diagnostic circuitry*** monitors the outputs of various components and circuits on the LTQ. Information on voltages, currents, temperatures, flow rates, logic, etc. is sent to the data system, where it can be accessed via diagnostics views of Tune Plus.

RF / Waveform Voltage Generation Electronic Assemblies

The ***RF/waveform voltage generation electronic assemblies*** produce the RF voltages for the mass analyzer, Q00 and Q0 quadrupoles, and Q1 octapole. They also produce the ion isolation waveform voltage, resonance excitation RF voltage, and resonance ejection RF voltage that are applied to the exit rods of the mass analyzer.

The main RF voltage generation involves the following components:

- RF oscillator
- RF Voltage Amplifier PCB
- Low Pass Filter PCB
- RF voltage coil
- RF voltage detector
- Mass DAC
- Integrating amplifier

The ***RF oscillator*** on the Digital PCB provides a 1.2 MHz sine wave reference signal that it uses to produce the RF voltage.

The ***RF Voltage Amplifier PCB*** produces the RF primary voltage for the RF voltage coil. To produce the RF primary voltage, the RF Voltage Amplifier PCB takes the sine wave reference signal and amplifies it by an amount based on a 0 to 10 V dc RF modulation signal from the integrating amplifier.

The ***Low Pass Filter PCB*** removes second and third harmonics from the RF primary voltage.

The ***RF voltage coil*** amplifies the RF primary voltage to produce a secondary voltage of 0 to 10,000 V ac (peak to peak) that is supplied to the rods of the mass analyzer.

The ***RF voltage detector*** senses the 0 to 10,000 V RF voltage signal applied to the rods of the mass analyzer and converts this sensed signal into a 0 to -10 V dc output signal.

The ***integrating amplifier*** (also called an error amplifier) produces the 0 to 10 V dc RF modulation signal that is used by the RF Voltage Amplifier PCB. The magnitude of the RF modulation signal is proportional to the difference between the detected RF signal and the mass set signal requested by the ***Mass DAC*** (digital-to-analog converter). The integrating amplifier adjusts the RF modulation signal until the detected RF signal equals the requested RF signal.

The ***Waveform DDS (direct digital synthesizer)***, which is part of the Digital PCB, provides the reference waveforms that are used to create the ion isolation waveform voltage, resonance excitation RF voltage, and resonance ejection RF voltage. The reference waveforms are amplified by a waveform amplifier on the Analog PCB. The amplified waveforms are then passed through the low pass filter, and they are finally combined at the RF voltage coil with the main RF for the exit rods.

The ***embedded computer***, which is also part of the Digital PCB, is where the computations that are required to produce the waveforms take place.

Ion Detection System Electronic Assemblies

The ***ion detection system electronic assemblies*** provide high voltage to the two electron multipliers and conversion dynodes of the ion detection system. They also receive the electron multiplier output current signal, convert it to a voltage (by the electrometer circuit), and pass it to the data system. A functional block diagram of the ion detection system electronic assemblies is shown in Figure 2-19.

The ion detection system electronic assemblies include the following:

- Electron multiplier/conversion dynode power supply
- Electrometer circuit

The ***electron multiplier/conversion dynode power supply*** supplies the -0.8 kV to -2.5 kV dc high voltage to the cathodes of the electron multipliers. The high voltage set control signal for the electron multiplier power supply comes from the Analog PCB. This signal controls a feedback control circuit and is proportional to the final high voltage to be applied to the electron multiplier cathode. The electron multiplier voltage is lowered by the Analog during sample ionization to prolong the life of the electron multiplier.

The electron multiplier/conversion dynode power supply also supplies +15 kV and -15 kV dc high voltage to the conversion dynode. The polarity of the voltage applied to the conversion dynode is determined by a control signal from the Analog PCB.

The ***electrometer circuit***, located in a shielded enclosure on the Electrometer PCB, receives the amplified ion current from the anodes of the electron multipliers, converts the current into a voltage, and then integrates the voltage over time. The integrated voltage is then passed to the Signal/Power Distribution PCB where it is processed and sent to the data system.

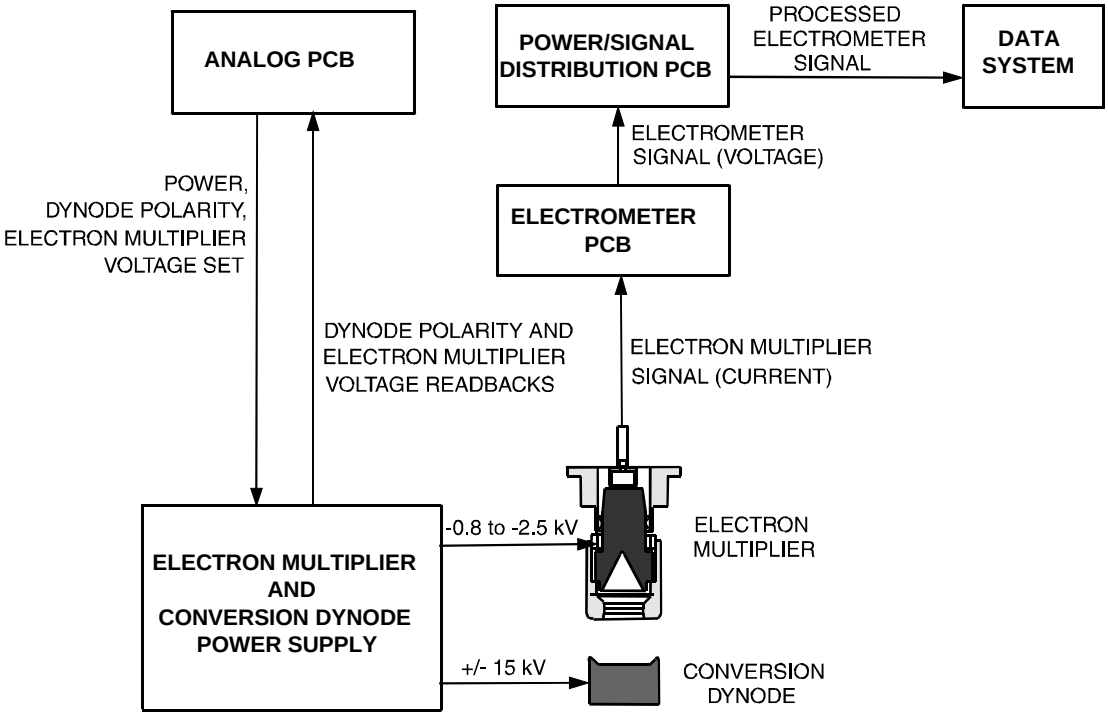


Figure 2-19. Functional block diagram of the ion detection system electronic assemblies

2.6 Data System

The ***data system*** controls and monitors the LTQ. The data system also processes data that is acquired by the LTQ. The data system is composed of the following:

- Computer hardware
- Data system/MS detector/LC interface
- Data system/local area network interface
- Printer (optional)

Computer Hardware

The data system computer has the following major features:

- Intel® Pentium® IV processor
- 512 MB of random access memory (RAM)
- High capacity hard disk drive
- Recordable/rewriteable CD drive
- Primary Ethernet adapter (data system to MS detector)
- Secondary Ethernet adapter (data system to local area network)
- 1.44-MB, 3.5-in. diskette drive
- Integrated video graphics card with 48 MB RAM
- 19-in., 1280 × 1024 resolution, flat panel LCD monitor
- Keyboard and mouse

For more information about the computer, refer to the manuals that come with the computer.

The minimum hardware and software requirements for the installation of Xcalibur 1.4 are:

- Intel Pentium III 500 MHz processor
- 256 MB RAM for processing
- 256 MB RAM for acquisition
- 6 GB hard drive (NTFS) or more recommended
- CD-ROM drive
- Video card and monitor capable of 1024 × 768 (XGA) resolution and 65,536 colors
- Microsoft Windows XP
- Microsoft Office XP

Data System / MS Detector / LC Interface

The data system computer contains a 100 base T Ethernet adapter (called the primary Ethernet adapter) that is dedicated to data system/MS detector/LC communications. This primary Ethernet adapter communicates with the MS detector, autosampler, and PDA detector via a 10/100 base T Ethernet switch. The Ethernet adapter on the MS detector resides on the on the Digital PCB.

Communication between the data system and the MS pump is established by way of an RS232 connection. A synchronization cable assembly is used to coordinate the run control signals between the LC modules and the MS detector. Refer to **Finnigan LTQ Getting Connected** for information on connecting the LTQ with other LC modules.

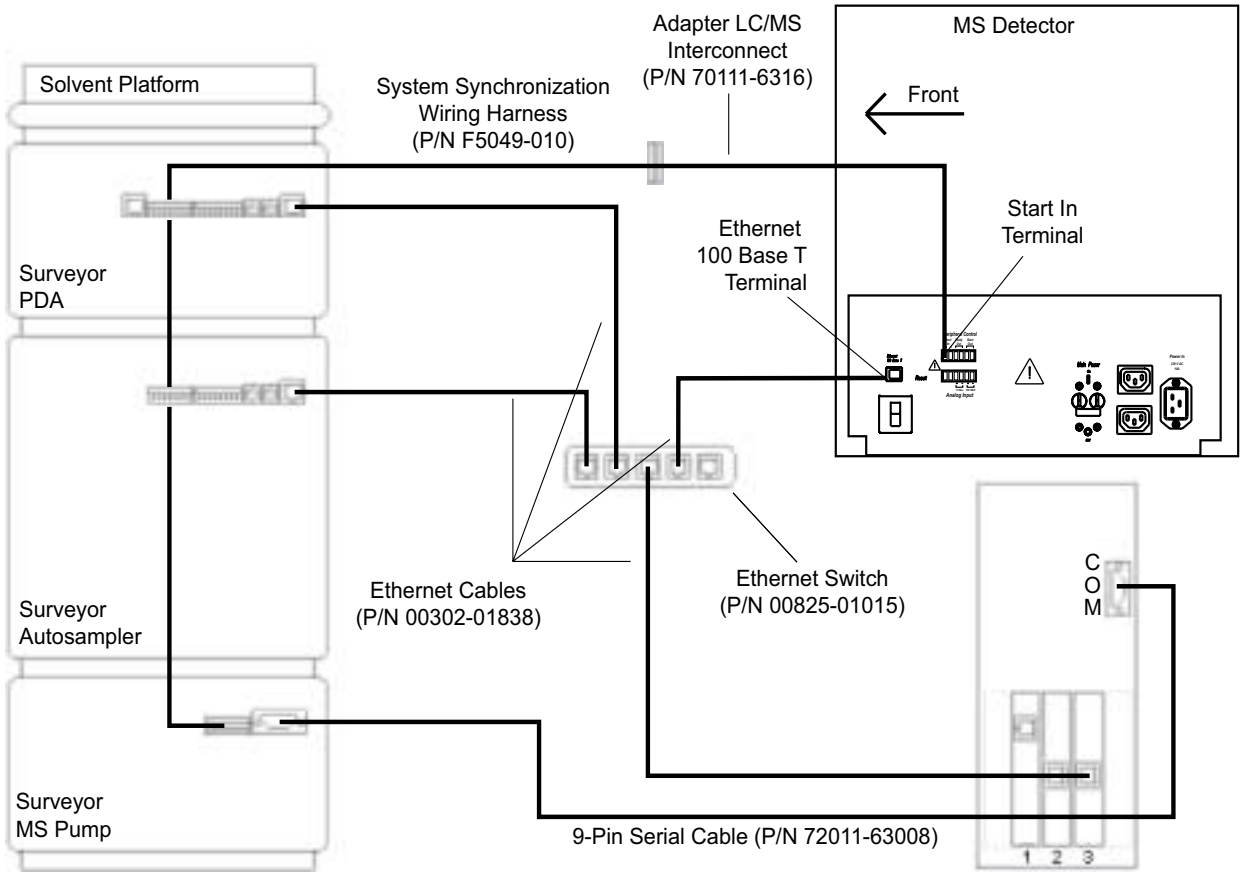


Figure 2-20. Cable diagram for the Surveyor LC system with an MS pump, LTQ MS detector, and data system computer

Data System / Local Area Network Interface

The data system computer contains a secondary Ethernet adapter. This secondary Ethernet adapter is not involved in data system/MS detector or LC communications. You can use this secondary Ethernet adapter to access your local area network.

Printer

A high-resolution laser printer is available with the LTQ as an option. The printer communicates with the PC via the local area network. Refer to the manual supplied by the manufacturer for details about the printer.

You set up the printer from the Print Setup dialog box. To open the Print Setup dialog box, choose **File > Print Setup** in any window.

Chapter 3
Daily Operation

This chapter outlines the checks and cleaning procedures of the LTQ system that should be performed every day to insure the proper operation of your system. This chapter is organized as follows:

- Things to do before operating the LTQ
- Things to do after operating the LTQ

Note. You do not need to tune and calibrate the LTQ as part of your daily routine.

Calibration parameters are instrument parameters that affect the mass accuracy and resolution. ***Tune parameters*** are instrument parameters that affect the intensity of the ion signal. You need to tune and calibrate the LTQ (that is, optimize the tune and calibration parameters) perhaps once a quarter. Refer to the **Automatic Tuning and Calibrating in the ESI/MS Mode** chapter in **Finnigan LTQ Getting Started** for a procedure for tuning and calibrating the LTQ. To check the tuning and calibration, follow the procedure described in the topic **Testing the Operation of the MS Detector in the ESI/MS Mode** in **Finnigan LTQ Getting Started**.

You need to optimize the tune parameters (or change the Tune Method) whenever you change the type of experiment. Refer to the **Optimizing the MS Detector with Your Compound in ESI/MS Mode** or **Optimizing the MS Detector with Your Compound in APCI/MS Mode** chapter in **Finnigan LTQ Getting Started** for a procedure for optimizing the tune parameters for your ESI or APCI experiment.

3.1 Things to Do Before Operating the LTQ

The following checks should be performed every day before you begin your first analysis:

- Check helium and nitrogen gas pressures
- Check the ESI fused-silica sample tube for elongation
- Check system vacuum levels
- Check disk space on the data system

Checking the Helium and Nitrogen Supplies

Check the helium supply on the regulator of the gas tank. Make sure that you have sufficient gas for your analysis. If necessary, install a new tank of helium. Verify that the pressure of helium reaching the MS detector is between 200 and 350 kPa (30 to 50 psig). If necessary, adjust the pressure with the tank pressure regulator.

Check the nitrogen supply on the regulator of the nitrogen gas tank or liquid nitrogen boil-off tank. Make sure that you have sufficient gas for your analysis. Typical nitrogen consumption is 100 cubic feet per day (nitrogen on 24 hours per day). If necessary, replace the tank. Verify that the pressure of nitrogen reaching the MS detector is between 550 and 830 kPa (80 to 120 psig). If necessary, adjust the pressure with the tank pressure regulator..

> **Note.** Before you begin normal operation each day, ensure that you have sufficient nitrogen for your API source. The presence of oxygen in the ion source when the MS detector is On could be unsafe. LTQ displays a popup message if the nitrogen pressure is too low.

Go on to the next topic: **Checking the ESI Fused-Silica Sample Tube for Elongation**.

Checking the ESI Fused-Silica Sample Tube for Elongation

Using acetonitrile in the mobile phase can cause elongation of the polyimide coating on the fused-silica sample tube. Elongation of the polyimide coating can degrade signal intensity and signal stability over time.

If you are running in ESI mode with a fused-silica sample tube, verify the sample tube is not elongated past the tip of the ESI spray needle.

Cut and reposition the end of the sample tube 1 mm inside the end of the ESI needle as follows:

1. Remove the ESI probe from the Ion Max ion source by following the procedure described in the section **Removing the ESI Probe** on page 2-7 of the **Finnigan Ion Max API Source Hardware Manual**.
2. Loosen the sample inlet fitting.
3. Gently pull back on the sample tube to free it from the fitting.
4. Push the sample tube forward so that it extends beyond the end of the electrospray needle.
5. Use a fused-silica cutting tool to cut off a small length of sample tube. Ensure that you cut the end of the sample tube squarely.
6. Pull the sample tube backwards until the exit end of the sample tube is recessed just inside the ESI needle by approximately 1 mm.
7. Tighten the sample inlet fitting securely to hold the sample tube in place.

> **Note.** The sample tube might move forward when you tighten the sample inlet fitting. Ensure that the sample tube is retracted into the ESI needle approximately 1 mm. If necessary, loosen the fitting and reposition the sample tube.

8. Reinstall the ESI probe as described in the section **Installing the ESI Probe** on page 2-9 of the **Finnigan Ion Max API Source Hardware Manual**.

Go on to the next topic: **Checking the System Vacuum Levels**.

Checking the System Vacuum Levels

For proper performance, your LTQ system must operate at the proper vacuum levels. Operation of the system with poor vacuum levels can cause reduced sensitivity, tuning problems, and reduced lifetime of the electron multiplier. You should check your system for air leaks by checking the system vacuum levels before you begin your first acquisition.

> **Note.** Major air leaks are often identifiable merely by listening for a rush of air or a hissing sound somewhere on the instrument. A major leak might be caused, for example, by a loose or disconnected fitting, by an O-ring that is not properly seated, or by an open valve.

You can check the current values of the pressures in the capillary-skimmer region and foreline (labeled *Convectron Gauge Pressure*) and in the analyzer region (labeled *Ion Gauge Press*) in the Vacuum dialog box of the Tune Plus window. To display the Tune Plus window choose **Start > Programs > Xcalibur > LTQ Tune**. Choose **Setup > Vacuum** to display the Vacuum dialog box.

Compare the current values of the pressures in the vacuum manifold with the values listed in Table 3-1. If the current values are higher than normal, you may have an air leak.

Table 3-1. Typical Pressure Readings

Conditions	Convectron gauge reading (foreline, capillary skimmer region)	Ion gauge reading (analyzer region)
Ion transfer capillary orifice open, ion transfer capillary at 250 °C	1.0 to 1.5 Torr	0.75×10^{-5} to 1.5×10^{-5} Torr

If the pressure is high (above 5×10^{-5} Torr in the analyzer region), and you have restarted the system within the last 30 to 60 minutes, wait an additional 30 minutes and recheck the pressure. If the pressure is decreasing with time, check the pressure periodically until it is within the typical pressure range of the MS detector.

If the pressure remains high, your system may have an air leak. If you suspect an air leak, shut down the system as described in the topic **Shutting Down the System Completely** on page 6-4. Make a visual inspection of the vacuum system and vacuum lines for leaks. Check each fitting and flange on the system for tightness, and tighten the fittings or flanges that are loose. Do not tighten fittings indiscriminately. Pay particular attention to fittings that have been changed recently or to fittings that have been subjected to heating and cooling. Make sure that the cover plates of the vacuum manifold are properly seated.

Go on to the next topic: **Checking the Disk Space.**

Checking the Disk Space

Periodically you should verify that your hard disk drive has enough free space for data acquisition. The amount of available disk space is shown in the Disk Space dialog box. To determine the amount of available disk space, proceed as follows:

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

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

3.2 Things to Do After Operating the LTQ

After operating the LTQ you need to do the following:

- Flush the sample transfer line, sample tube, and API probe
- Place the system in standby condition
- Flush the ion sweep cone and ion transfer capillary
- Purge the oil in the rotary-vane pump
- Empty the solvent waste bottle

Flushing the Sample Transfer Line, Sample Tube, and API Probe

You should flush the sample transfer line, sample tube, and API probe at the end of each working day (or more often if you suspect they are contaminated) by flowing a 50:50 methanol:distilled water solution from the LC through the API source.

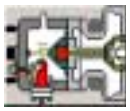
To flush the sample transfer line, sample tube, and API probe, proceed as follows:

1. Wait until data acquisition, if any, is complete.
2. Make sure that the lid to the API chamber in closed and secured.
3. Choose **Start > Programs > Xcalibur > LTQ Tune** to open the LTQ Tune Plus window.


On


Standby

4. From the Tune Plus window, choose **Control > On** (or click on the On/Standby button to toggle it to On) to turn on the voltages and gas flows to the API source.
   - If you are operating in APCI or APPI mode, go to step 5.
   - If you are operating in ESI mode, go to step 6.
5. Set up the APCI source as follows:



   a. In the LTQ Tune Plus window, choose **Setup > APCI Source** to (or click on the APCI source button) to display the APCI Source dialog box.

   b. Set the APCI vaporizer temperature to 500 °C:
   In the APCI Source dialog box, enter **500** in the Vaporizer Temperature text box.

   c. Set the sheath gas flow rate to 30:
   In the APCI Source dialog box, enter **30** in the Sheath Gas Flow Rate text box.

d. Set the auxiliary gas flow rate to 5:
In the APCI Source dialog box, enter **5** in the Aux Gas Flow Rate text box.

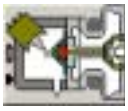
e. Set the sweep gas flow rate to 0:
In the APCI Source dialog box, enter **0** in the Sweep Gas Flow Rate text box.

f. Set the APCI spray current to 0:
In the APCI Source dialog box, enter **0** in the Spray Current text box.

g. Click on **OK**.

Go to step 7.

6. Set up the ESI source as follows:



a. In the LTQ Tune Plus window, choose **Setup > ESI Source** to (or click on the ESI source button) to display the ESI Source dialog box.

b. Set the sheath gas flow rate to 30:
In the ESI Source dialog box, enter **30** in the Sheath Gas Flow Rate text box.

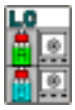
c. Set the auxiliary gas flow rate to 5:
In the ESI Source dialog box, enter **5** in the Aux Gas Flow Rate text box.

d. Set the sweep gas flow rate to 0:
In the ESI Source dialog box, enter **0** in the Sweep Gas Flow Rate text box.

e. Set the ESI spray voltage to 0:
In the ESI Source dialog box, enter **0** in the Spray Voltage text box.

f. Click on **OK**.

7. Set up and start a flow of 50:50 methanol:water solution from the LC to the API source, as follows:



a. In the LTQ Tune Plus window, choose **Setup > Inlet Direct Control** (or click on the AS/LC direct control button). The Inlet Direct Control view appears.

b. Select the LC tab.

c. Set the Flow Rate to a value that is typical for your experiments.

d. Set the solvent proportions to 50% methanol and water.

e. Click on  (or **Pump On** or **Start Pump)** to start the LC pump.

8. Let the solution flow through the sample transfer line, sample tube, and API probe for 15 min. After 15 min, turn off the flow of liquid from the LC to the API source, as follows. Leave the API source (including the APCI vaporizer, sheath gas, and auxiliary gas) on for an additional 5 min. Click on  (or **Pump Off** or **Stop Pump)** to stop the LC pump.

9. After 5 min, turn off the API source by placing the MS detector in Standby: From the LTQ Tune Plus window, choose **Control > Standby** (or click on the On/Standby button) to put the MS detector in Standby.

Go on to the next topic: **Placing the System in Standby Condition**.

Placing the System in Standby Condition

Use the following procedure to place the LTQ system in the standby condition:


On


Standby

1. From the LTQ Tune Plus window, choose **Control > Standby** (or click on the On/Standby button) to put the MS detector in Standby. The System LED on the front panel of the MS detector is illuminated yellow when the system is in Standby.
2. Leave the MS detector power on.
3. Leave the LC power on.
4. Leave the autosampler power on.
5. Leave the data system power on.

Go on to the next topic: **Flushing the Ion Sweep Cone and Ion Transfer Capillary**.

Flushing the Ion Sweep Cone and Ion Transfer Capillary

You need to clean the ion sweep cone (or spray cone) and the ion transfer capillary on a regular basis to prevent corrosion and to maintain optimum performance of your API source. A good practice is to flush the ion sweep cone and ion transfer capillary at the end of each operating day after you flush the sample transfer line, sample tube, and API probe with a 50:50 methanol:water solution from the LC. (Refer to the topic **Flushing the Sample Transfer Line, Sample Tube, and API Probe** on page 3-6.) If you are operating the system with nonvolatile buffers in your solvent system or high concentrations of sample, you might need to clean the ion sweep cone and ion transfer capillary more often.

You do not need to vent the system to flush the ion sweep cone and ion transfer capillary. To clean the ion sweep cone and the ion transfer capillary, do the following:

1. Turn off the flow of liquid from the LC (or other sample introduction device) to the API source. To turn off the flow of liquid from the LC to the API source, do the following:
   a. Choose **Start > Programs > Xcalibur > LTQ Tune** to open the LTQ Tune Plus window.

b. In the LTQ Tune Plus window, choose **Setup > Inlet Direct Control** (or click on the AS/LC direct control button). The Inlet Direct Control view appears.

c. Select the LC tab and click on  (or **Pump Off** or **Stop Pump)** to stop the LC pump.

2. From the LTQ Tune Plus window, choose **Control > Standby** (or click on the On/Standby button) to put the MS detector in Standby.

3. Open the door of the Ion Max ion source.

CAUTION. AVOID BURNS. At operating temperatures, the APCI vaporizer and ion transfer capillary can severely burn you! The APCI vaporizer typically operates at 400 to 600 °C and the ion transfer capillary typically operates at 100 to 300 °C. Allow the heated vaporizer and ion transfer capillary to cool to room temperature, for approximately 20 min, before you touch or remove either component.

4. Fill a spray bottle with a 50:50 solution of HPLC-grade methanol:distilled water. Spray approximately 5 mL of the solution at the opening of the ion transfer capillary. Do not touch the ion transfer capillary with the tip of the spray bottle.

5. Use the spray bottle filled with the 50:50 solution of methanol:water to flush contaminants from the accessible surfaces of the ion source chamber and the spray cone or ion sweep cone (if it is installed).

6. Ensure that you have removed any salt or other contaminants that may have been deposited on the ion sweep cone or spray cone. If necessary, remove the Ion Max ion source and clean the ion sweep cone or spray cone as follows:

   a. Remove the Ion Max ion source from the front of the MS detector as described in the topic **Removing the Ion Max Ion Source** on page 4-12.

   b. Remove the ion sweep cone (if it is installed) as follows:

      i. Put on a pair of talc-free gloves.

      ii. Grasp the outer ridges of the ion sweep cone and pull the cone straight off of the API cone seal. Note, you might need to loosen the set screws on the ion sweep cone in order to remove it.

Note. This is a good point to remove and clean the ion transfer capillary. You remove the ion transfer capillary by unsrewing it counter clockwise with the custom removal tool. Refer to topic **Removing and Cleaning the Ion Transfer Capillary** on page 4-8.

   c. Clean the ion sweep cone as follows:

i. Place the ion sweep cone and the ion capillary tube in a beaker of 50:50 methanol/water.

ii. Sonicate it for 15 min.

iii. Dry the ion sweep cone.

d. Clean the spray cone with a Kimwip soaked in methanol.

e. Reinstall the ion sweep cone as follows:

i. Note the location of the sweep gas supply port in the API cone seal. The gas inlet on the ion sweep cone is placed in this port. See Figure 3-1 and Figure 3-2.

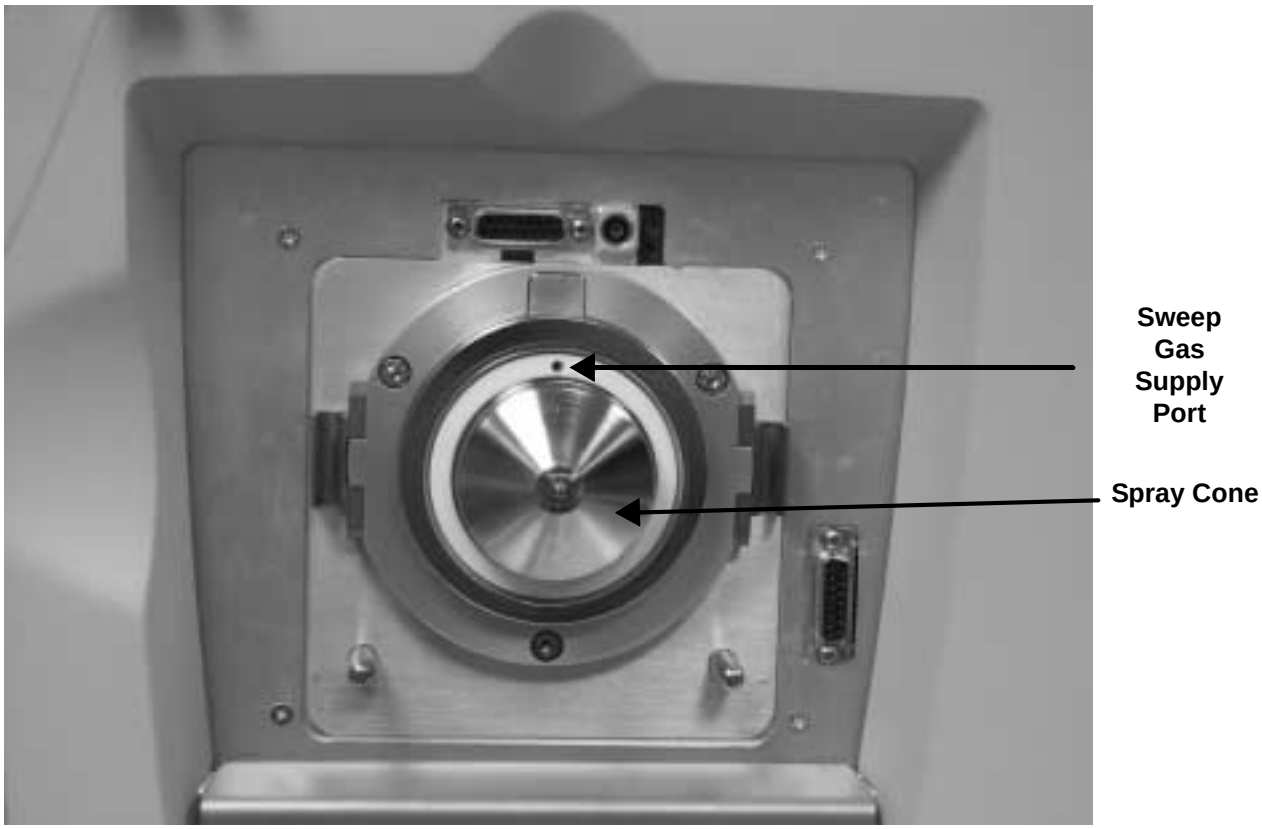


Figure 3-1. Sweep gas supply port in the API cone seal

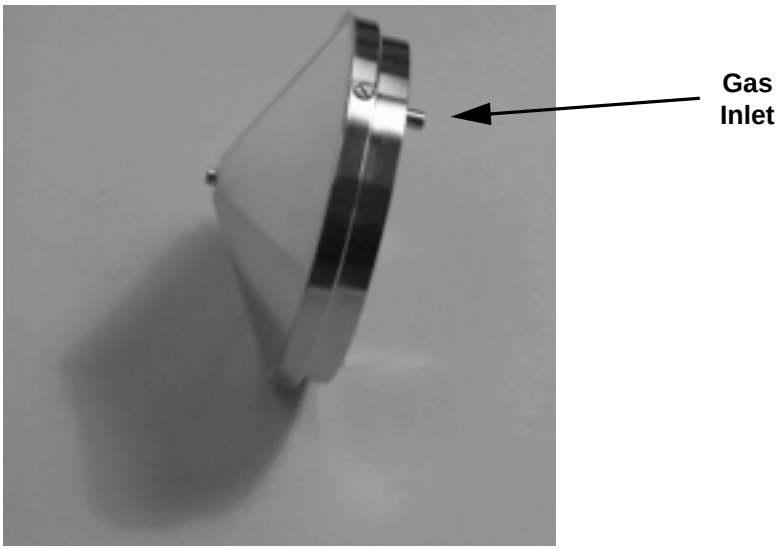


Figure 3-2. Ion sweep cone, showing the gas inlet

ii. Carefully align the gas inlet on the ion sweep cone with the sweep gas supply port in the API cone seal. Firmly press the ion sweep cone into position.

iii. If necessary to achieve a proper ion sweep cone installation, you might adjust the set screws around the perimeter of the ion sweep cone.

f. Reinstall the Ion Max ion source as described in the topic **Reinstalling the Ion Max Ion Source** on page 4-19.

Go on to the next topic: **Purging the Oil in the Rotary-Vane Pump**.

Purging the Oil in the Rotary-Vane Pump

You need to purge (decontaminate) the oil in the rotary-vane pump on a daily basis to remove water and other dissolved chemicals from the pump oil. Water and other chemicals in the rotary-vane pump can cause corrosion and decrease the lifetime of the pump. A good time to purge the oil is at the end of the working day after you flush the API probe, ion sweep cone, and ion transfer capillary.

To purge the oil in the rotary-vane pump, proceed as follows:

1. Turn off the flow of liquid from the LC (or other sample introduction device) to the API source. To turn off the flow of liquid from the LC to the API source, do the following:

   a. Choose **Start > Programs > Xcalibur > LTQ Tune** to open the LTQ Tune Plus window.

b. In the LTQ Tune Plus window, choose **Setup > Inlet Direct Control** (or click on the AS/LC direct control button). The Inlet Direct Control view appears.

c. Select the LC tab and click on  (or **Pump Off** or **Stop Pump)** to stop the LC pump.


On


Standby

2. From the LTQ Tune Plus window, choose **Control > Standby** (or click on the On/Standby button) to put the MS detector in Standby. Ensure that a septum seals the entrance to the ion transfer capillary.
3. Open the gas ballast valve on the rotary-vane pump by turning it to position **|**. Refer to the manual that came with the pump for the location of the gas ballast valve.
4. Allow the pump to run for 30 min with the gas ballast valve open.
5. After 30 min, close the gas ballast valve by turning it to position O.

Go on to the next topic: **Emptying the Solvent Waste Bottle**.

Emptying the Solvent Waste Bottle

The solvent level in the solvent waste bottle should be checked on a daily basis. If necessary, empty the solvent waste bottle. Dispose of the solvent waste in accordance with local and federal regulations.

Chapter 4
MS Detector Maintenance

LTQ performance depends on the maintenance of all parts of the instrument. **It is your responsibility to maintain your system properly by performing the system maintenance procedures on a regular basis**.

This chapter describes routine MS detector maintenance procedures that must be performed to ensure optimum performance of the instrument. Most of the procedures involve cleaning. For example, procedures are provided for cleaning the API source, ion guides, mass analyzer, and ion detection system. Procedures are also presented for replacing the API sample tube, ion transfer capillary, and API source, ion optics, and mass analyzer assemblies.

Routine and less frequent MS detector maintenance procedures are listed in Table 4-1.

Table 4-1. MS detector maintenance procedures

MS Detector Component	Procedure	Frequency	Procedure Location
API source	Flush (clean) sample transfer line, sample tube, and API probe	Daily	Page 3-6
Ion source interface	Flush (clean) ion sweep cone and ion transfer capillary	Daily (or more often[1])	Page 3-8
Rotary-vane pump	Purge (decontaminate) oil	Daily	Page 3-11
Ion source interface	Remove and clean ion transfer capillary	Weekly, or if ion transfer capillary bore is contaminated or obstructed	Page 4-8
PhotoMate light source	Clean or polish VUV lamp window	If VUV lamp window is dirty	**Finnigan Ion Max API Source Hardware Manual**
Ion source interface	Clean tube lens and skimmer	As needed[1]	Page 4-13
Cooling fans	Clean fan filters	Every 4 months	Page 4-44
Q00 ion guide	Clean Q00 quadrupole and lens L0	As needed[1]	Page 4-22
ESI probe	Trim sample tube	If polyimide coating on the end of the sample tube has elongated	Page 3-3
APCI or ESI probe	Replace sample tube	If sample tube is broken or obstructed	**Finnigan Ion Max API Source Hardware Manual**
Ion source interface	Replace ion transfer capillary	If ion transfer capillary bore is corroded	**Finnigan Ion Max API Source Hardware Manual**
PhotoMate light source	Replace VUV lamp	If lamp fails	**Finnigan Ion Max API Source Hardware Manual**
Q0 ion guide	Clean Q0 quadrupole and intermultiple lens L1[2]	As needed[1]	Page 4-28
Q1 ion guide	Clean Q1 octapole and gate lens[2]	As needed[1]	Page 4-28

Table 4-1. MS detector maintenance procedures, continued

MS Detector Component	Procedure	Frequency	Procedure Location
Ion detection system	Clean ion detection system (electron multiplier and conversion dynode)	Whenever the top cover plate of the vacuum manifold is removed	Page 4-36
Mass analyzer	Clean mass analyzer[2]	Very rarely (if ever)[1]	Page 4-38
Rotary-vane pump	Add oil	If oil level is low	Manufacturer's documentation
Rotary-vane pump	Change oil	Every 3 months or if oil is cloudy or discolored	Manufacturer's documentation
Ion detection system	Replace electron multiplier assembly[2]	If noise in spectrum is excessive or proper electron multiplier gain can not be achieved	Page 4-39
Turbomolecular pump	Replace turbomolecular pump insert[2]	Every 20,000 to 30,000 hours or if bearings fail	Page 4-43
Electronic modules	Replace electronic module[2]	If electronic module fails	**Diagnostics and PCB and Assembly Replacement** chapter
PCBs	Replace PCB[2]	If PCB fails	**Diagnostics and PCB and Assembly Replacement** chapter

[1]Frequency depends on analytical conditions

[2]We recommend that this maintenance procedure be performed by a Thermo Electron Field Service Engineer

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

The topics included in this chapter are as follows:

- Tools and supplies
- Frequency of cleaning
- API source maintenance
- Cleaning the Q00 ion guide
- Cleaning the Q0 ion guide
- Cleaning the mass analyzer
- Cleaning the ion detection system
- Replacing the electron multiplier
- Replacing the turbomolecular pump insert
- Cleaning the fan filters

Note. The keys to success with the procedures in this chapter are:

- Proceed methodically.
- Always wear clean, lint-free gloves when handling the components of the API source, ion guides, mass analyzer, and ion detection system.
- Always place the components on a clean, lint-free surface.
- Never overtighten a screw or use excessive force.

4.1 Tools and Supplies

The LTQ requires very few tools for you to perform routine maintenance procedures. You can remove and disassemble many of the components by hand. The tools, equipment, and chemicals listed in Table 4-2 are needed for the maintenance of the API source, ion guides, mass analyzer, and ion detection system.

Table 4-2. Tools, equipment, and chemicals

Description	Part Number
Screwdrivers, set, ball point, Allen (also referred to as ball drivers)	00025-03025
Hex ball Driver, 3/16-in.	00025-01700
Hex ball Driver, 7/64-in.	00025-01800
Hex ball driver, 5/16-in., 9.5 in. long	00025-10015
Hex ball driver, 5/32, 7.4 in. long	00025-10020
Ion transfer capillary removal tool	70111-20258
Screwdriver, slot head, large	
Screwdriver, slot head, small	
Screwdriver, Phillips, small	
Fused-silica cutting tool	
Spray bottle	
Beaker, 450 mL	
Gloves, nylon	00301-09700
Kimwipes or other lint-free industrial tissue	
Applicators (swabs), cotton-tipped	00301-02000
Detergent	
Clean, dry, compressed nitrogen gas	
Distilled water	
Methanol, HPLC grade or better	
Nitric acid, dilute	

CAUTION. As with all chemicals, solvents and reagents should be stored and handled according to standard safety procedures and should be disposed of according to local and federal regulations.

4.2 Frequency of Cleaning

The frequency of cleaning the components of the MS detector depends on the types and amounts of samples and solvents that are introduced into the instrument. In general, for a given sample and ionization technique, the closer a MS detector component is to the source of the ions, the more rapidly it becomes dirty.

- The sample tube, API probe, ion transfer capillary bore, and ion sweep cone of the API source should be cleaned at the end of each operating day to remove any residual salts from buffered mobile phases or other contamination that might have accumulated during normal operation. Refer to the topics **Flushing the Sample Transfer Line, Sample Tube, and API Probe** on page 3-7 and **Flushing the Ion Sweep Cone and Ion Transfer Capillary** on page 3-9.
- The tube lens and skimmer of the Q00 ion guide become dirty at a slower rate than the API probe, ion sweep cone, and ion transfer capillary. The Q00 quadrupole and lens L0 require cleaning less often than the tube lens and skimmer. Refer to the topic **Cleaning the Q00 Ion Guide** on page 4-22.
- The Q0 quadrupole, Q1 octapole, and lenses of the Q0 and Q1 ion guides become dirty at a rate significantly slower than the API source and Q00 ion guide. Refer to the topic **Cleaning the Q0 and Q1 Ion Guides** on page 4-28.
- The quadrupoles of the mass analyzer require cleaning very rarely (if ever). Refer to the topic **Mass Analyzer Maintenance** on page 4-38.
- Clean the electron multiplier and conversion dynode whenever you remove the top cover plate of the vacuum manifold by blowing them with a clean, dry gas. Refer to the topic **Cleaning the Ion Detection System** on page 4-36.

When the performance of your system decreases significantly due to contamination, clean the components of the MS detector in the following order:

- Clean the API probe, ion sweep cone (if it is installed), spray cone, and ion transfer capillary
- Clean the tube lens and skimmer
- Clean the quadrupole and lens of the Q00 ion guide
- Clean the quadrupole and lens of the Q0 ion guide and the octapole and lens of the Q1 ion guide
- Clean the mass analyzer

4.3 API Source Maintenance

The API source requires a minimum of maintenance. Periodically, you need to clean the components of the API source to remove salts or other contaminants. The frequency of cleaning the API source depends on the types and amounts of samples and solvents that are introduced into the instrument.

Maintenance procedures are provided below to do the following:

- Flush the sample transfer line, sample tube, and API probe
- Flush the ion sweep cone (or spray cone) and the bore of the ion transfer capillary
- Remove and clean the ion transfer capillary
- Maintain the API probes, including replacing the sample tube
- Maintain the PhotoMate light source, including replacing the VUV lamp
- Maintain the ion source interface, including replacing the ion transfer capillary and heater

CAUTION. AVOID EXPOSURE TO POTENTIALLY HARMFUL MATERIALS. Always wear protective gloves and safety glasses when you use solvents or corrosives. Also, contain waste streams and use proper ventilation. Refer to your supplier's Material Safety Data Sheets (MSDS) for procedures that describe how to handle a particular solvent.

Flushing the Sample Transfer Line, Sample Tube, and API Probe

You should flush the sample transfer line, sample tube, and API probe at the end of each working day (or more often if you suspect they are contaminated) by flowing a 50:50 methanol:distilled water solution from the LC through the API source.

To flush the sample transfer line, sample tube, and API probe, follow the procedure described in the topic **Flushing the Sample Transfer Line, Sample Tube, and API Probe** on page 3-6.

Flushing the Ion Sweep Cone and Ion Transfer Capillary

You need to clean the ion sweep cone (or the spray cone, if the ion sweep cone is not installed) and the ion transfer capillary on a regular basis to prevent corrosion and to maintain optimum performance of your API source. A good practice is to flush the ion sweep cone and ion transfer capillary at the end of each operating day after you flush the sample transfer line, sample tube, and API probe with a 50:50 methanol:water solution from the LC. To clean the ion

sweep cone and the ion transfer capillary follow the procedure described in the topic **Flushing the Ion Sweep Cone and Ion Transfer Capillary** on page 3-8.

Removing and Cleaning the Ion Transfer Capillary

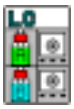
The bore of the ion transfer capillary can become blocked by buffer salts or high concentrations of sample. The ion transfer capillary can be easily removed for cleaning. You do not have to vent the system to remove the ion transfer capillary.

If the pressure in the ion transfer capillary-skimmer region (as measured by the Convectron gauge) drops considerably below 1 Torr, you should suspect a blocked ion transfer capillary. You can check the Convectron gauge pressure in the Vacuum dialog box of the Tune Plus window. To display the Tune Plus window choose **Start > Programs > Xcalibur > LTQ Tune**. Choose **Setup > Vacuum** to display the Vacuum dialog box.

To remove and clean the ion transfer capillary, do the following:

1. Turn off the flow of liquid from the LC (or other sample introduction device) to the API source. To turn off the flow of liquid from the LC to the API source, do the following:

   a. Choose **Start > Programs > Xcalibur > LTQ Tune** to open the Tune Plus window.

   b. In the LTQ Tune Plus window, choose **Setup > Inlet Direct Control** (or click on the AS/LC direct control button). The Inlet Direct Control view appears.

   c. Select the LC tab and click on  (or **Stop Pump** or **Pump Off**) to stop the LC pump.

2. Place the electronics service switch (located on the right side of the MS detector) in the Service position to turn off the non-vacuum system voltages.

CAUTION. Make sure that the LTQ electronics service switch is in the Service position before you proceed.

3. Remove the Ion Max ion source from the front of the MS detector as described in the topic **Removing the Ion Max Ion Source** on page 4-12.

CAUTION. The ion transfer capillary typically operates at 250 to 400 °C. Allow the ion transfer capillary and ion sweep cone to cool before you remove them.

4. Remove the ion sweep cone by grasping the outer ridges of the ion sweep cone and pull the cone straight off of the API cone seal. Note, you might need to loosen the set screws on the ion sweep cone in order to remove it. See Figure 4-1.
5. Remove the ion transfer capillary (P/N 97055-20198) by turning it counterclockwise with the custom removal tool (P/N 70111-20258) until you can pull it free from the ion source interface.
6. Soak the ion transfer capillary in a dilute solution of nitric acid to remove contaminants.
7. Sonicate the ion transfer capillary in distilled water.
8. Clean the ion sweep cone by wiping the inside and outside with methanol and a Kimwipe.
9. Remove, clean with methanol, and inspect the 0.3-in. ID Kalrez® O-ring (P/N 00107-12750) that seats in the spray cone under the entrance end of the ion transfer capillary. Replace it if necessary.

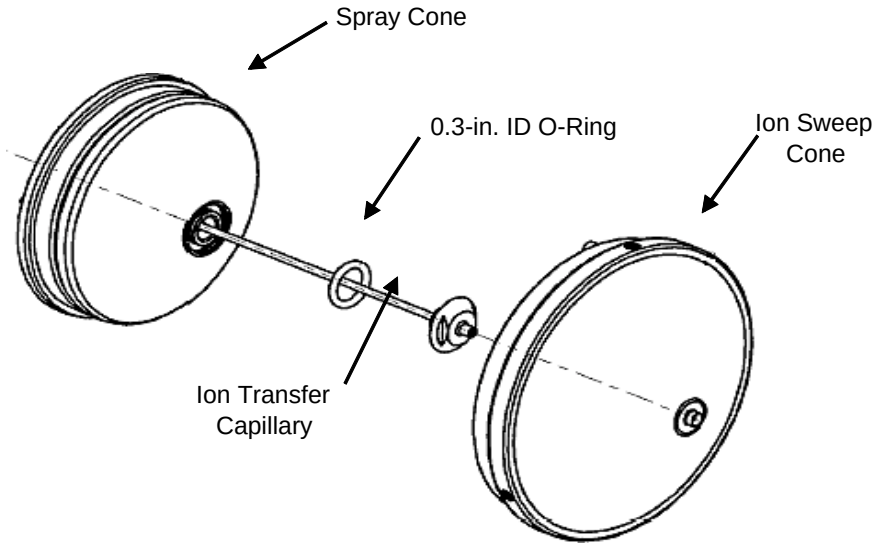


Figure 4-1. Ion sweep cone, ion transfer capillary, O-ring, and spray cone of the ion source interface

10. Reseat the O-ring in the spray cone.

> **Caution.** Be careful not to bend the ion transfer capillary. Rotate the capillary as you insert it.

11. Insert the ion transfer capillary into the heater block. Rotate the capillary as you insert it. Once inserted, turn the capillary clockwise until it is finger tight.
12. Reinstall the ion sweep cone on the ion source interface.
13. Reinstall the Ion Max ion source on the MS detector as described in the topic **Reinstalling the Ion Max Ion Source** on page 4-19.

> **Note.** If you have unblocked the ion transfer capillary, the Convectron gauge pressure should increase to a normal value (approximately 1 Torr). If you cannot clear the ion transfer capillary by this method, replace the ion transfer capillary.

14. Place the electronics service switch in the Electronics Normal position to turn on the non-vacuum system voltages.

Maintaining the API Probes

The API probes of the Ion Max ion source requires a minimum of maintenance. If the sample tube becomes obstructed with salt precipitates or is broken, you need to replace it. Also, you may need to disassemble an API probe so you can clean it or to replace a part.

Refer to the **Finnigan Ion Max API Source Hardware Manual** for procedures for maintaining the API probes.

> **Note.** You should flush the API probe at the end of each working day by flowing a 50:50 HPCL-grade methanol:distilled water solution from the LC through the APCI probe. Refer to the topic **Flushing the Sample Transfer Line, Sample Tube, and API Probe** on page 3-7.

Maintaining the PhotoMate Light Source

Maintaining the PhotoMate light source involves the following:

- Cleaning and polishing the VUV lamp
- Replacing the VUV lamp

Refer to the topic **Maintaining the APPI Probe** in the **Finnigan Ion Max API Source Hardware Manual** for procedures for maintaining the APPI probe.

Maintaining the Ion Source Interface

The ion source interface includes the ion sweep cone, ion transfer capillary, capillary heater, tube lens, and skimmer. The ion transfer capillary has a finite lifetime. You need to replace the ion transfer capillary if the ion transfer capillary bore becomes corroded.

You should flush the ion sweep cone and the bore of the ion transfer capillary at the end of each working day with a 50:50 methanol:water solution. Refer to the topic **Flushing the Ion Sweep Cone and Ion Transfer Capillary** on page 3-9.

The ion transfer capillary can be easily removed for cleaning or replacement without venting the system. Refer to the topic **Removing and Cleaning the Ion Transfer Capillary** on page 4-8.

To access the tube lens and skimmer for cleaning or to replace ion source interface components other than the ion transfer capillary and ion sweep cone, do the following:

- Shut down and vent the system
- Remove the Ion Max ion source
- Remove the ion source interface
- Clean or replace ion source interface components
- Reinstall the ion source interface
- Reinstall the Ion Max ion source
- Start up the system

Shutting Down the System

Shut down and vent the system as described in the topic **Shutting Down the System Completely** in the **System Shutdown, Startup, and Reset** chapter. Wait several minutes for the LTQ to vent.

Go on to the next topic: **Removing the Ion Max Ion Source**.

Removing the Ion Max Ion Source

You need to remove the Ion Max ion source to access the ion source interface and Q00 ion guide.

> **Note.** If an ion source probe is still installed in the ion source housing, the external liquid lines should first be disconnected before removing the ion source housing.

Remove the Ion Max ion source as follows:

1. Remove the drain tube from the ion source housing drain. See Figure 4-2.

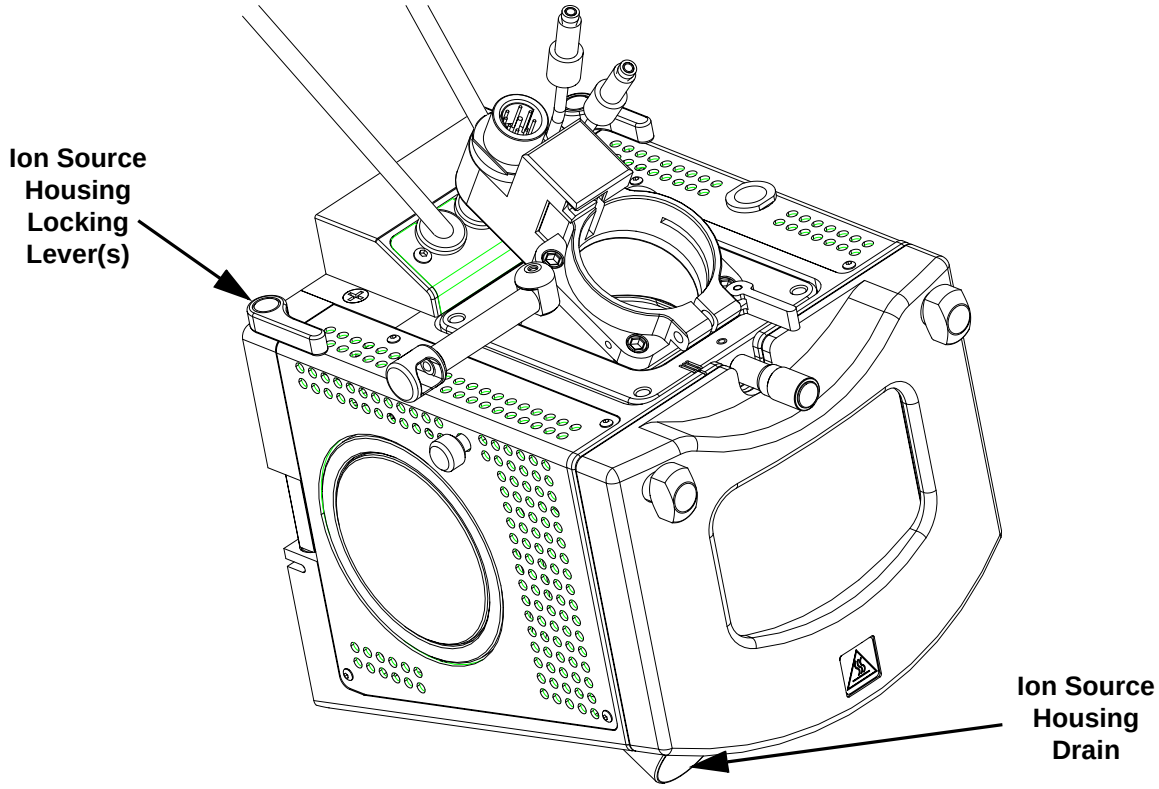


Figure 4-2. Ion Max ion source, showing the locking levers and drain

2. Rotate the ion source housing locking levers 90° to release the ion source housing from the ion source mount assembly.
3. Remove the ion source housing by pulling straight off of the ion source mount assembly, and place the housing in a safe location for temporary storage.

Go on to the next topic: **Removing the Ion Source Interface**.

Removing the Ion Source Interface

CAUTION. Make sure that the LTQ power cord is unplugged before you proceed.

To remove the ion source interface, grasp the ridges on either side of the ion source interface and carefully pull it free from the vacuum manifold. Place it on a clean surface.

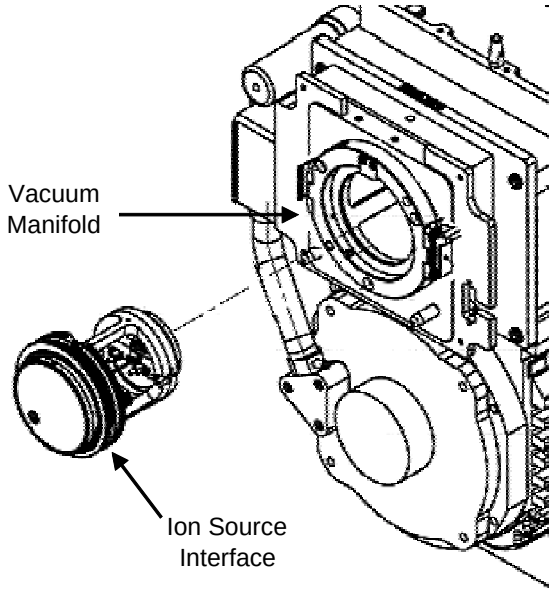


Figure 4-3. Ion source interface removal

To replace components of the ion source interface, go to the topic: **Replacing Ion Source Interface Components** on page 4-15.

To clean the tube lens and skimmer, go on to the next topic: **Cleaning the Tube Lens and Skimmer**.

Cleaning the Tube Lens and Skimmer

An accumulation of chemicals on the surfaces of the tube lens and skimmer forms an insulating layer that can modify the electrical fields that control ion transmission. The tube lens and skimmer require cleaning less often than the ion sweep cone and the ion transfer capillary.

To clean the tube lens and skimmer proceed as follows:

CAUTION. Wait for the ion source interface to cool to ambient temperature before you disassemble it.

Note. Wear clean gloves when you handle the tube lens and skimmer.

Caution. Take care not to scratch or nick the skimmer cone.

4. Remove the skimmer by carefully pulling it free from the rear of the ion source interface. Note the orientation of the skimmer.
5. Remove the tube lens by carefully pulling it free from the rear of the ion source interface. Note the orientation of the tube lens.

Note. For most cleaning applications, HPLC grade methanol is the solvent of choice. However, use of buffers or salt solutions may require that you use an acidic, aqueous solution. If you need to use a solvent other than methanol, after cleaning the component, flush the component with distilled water and then flush it with methanol as a final wash. In all cases, ensure that all solvent has evaporated from the component(s) before reassembly.

6. Clean the tube lens inside and out with HPLC-grade methanol and a cotton-tipped applicator (swab).
7. Clean the skimmer inside and out with HPLC-grade methanol and a cotton-tipped applicator (swab).

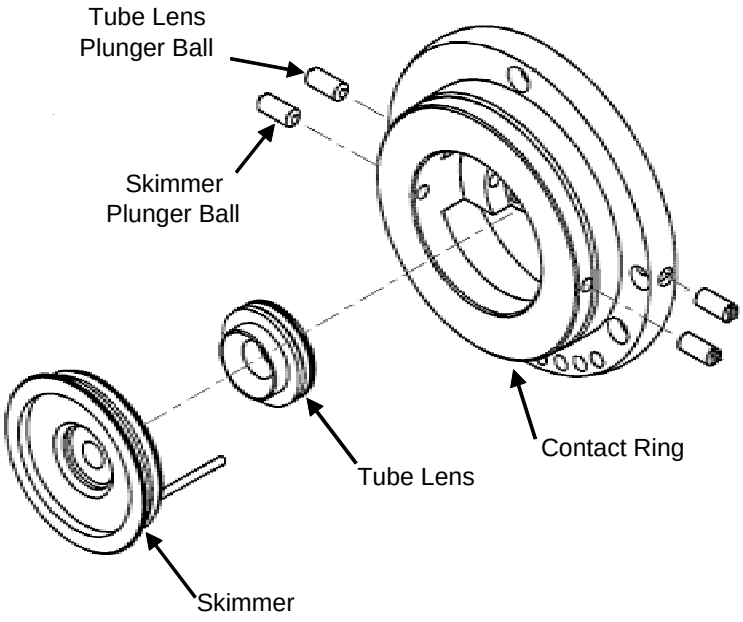


Figure 4-4. Rear of the ion source interface showing the tube lens and skimmer

8. Reinstall the tube lens in the ion source interface:
   a. Orient the tube lens such that the lead pin points toward the socket.
   b. Push the tube lens until it snaps into place.

> **Caution.** Take care not to scratch or nick the skimmer cone.

9. Reinstall the skimmer in the ion source interface:
   a. Orient the skimmer such that the lead pin points toward the socket.
   b. Push the skimmer until it snaps into place.

> **Note.** There are no leads to connect to the tube lens and skimmer.

Go on to the topic: **Reinstalling the Ion Source Interface** on page 4-19.

Replacing Ion Source Interface Components

> **CAUTION.** Wait for the ion source interface to cool to ambient temperature before you disassemble it.

> **Note.** Wear clean gloves when you handle the ion source interface components.

The capillary heater assembly must be replaced as a unit. To remove the capillary heater assembly proceed as follows:

1. Remove the ion transfer capillary by turning it counterclockwise until you can pull it free from the ion source interface.
2. Disconnect the capillary heater cable from the connector.
3. Disconnect the grounding wire.
4. Loosen the two screws that hold the capillary heater mount to the ion source interface housing.
5. Remove the capillary heater assembly.
6. To install a new capillary heater assembly (P/N 97055-20074), reverse steps 1 through 4.

To replace other ion source interface component, refer to the exploded diagrams shown in Figure 4-5 and Figure 4-6.

Go on to the next topic: **Reinstalling the Ion Source Interface**.

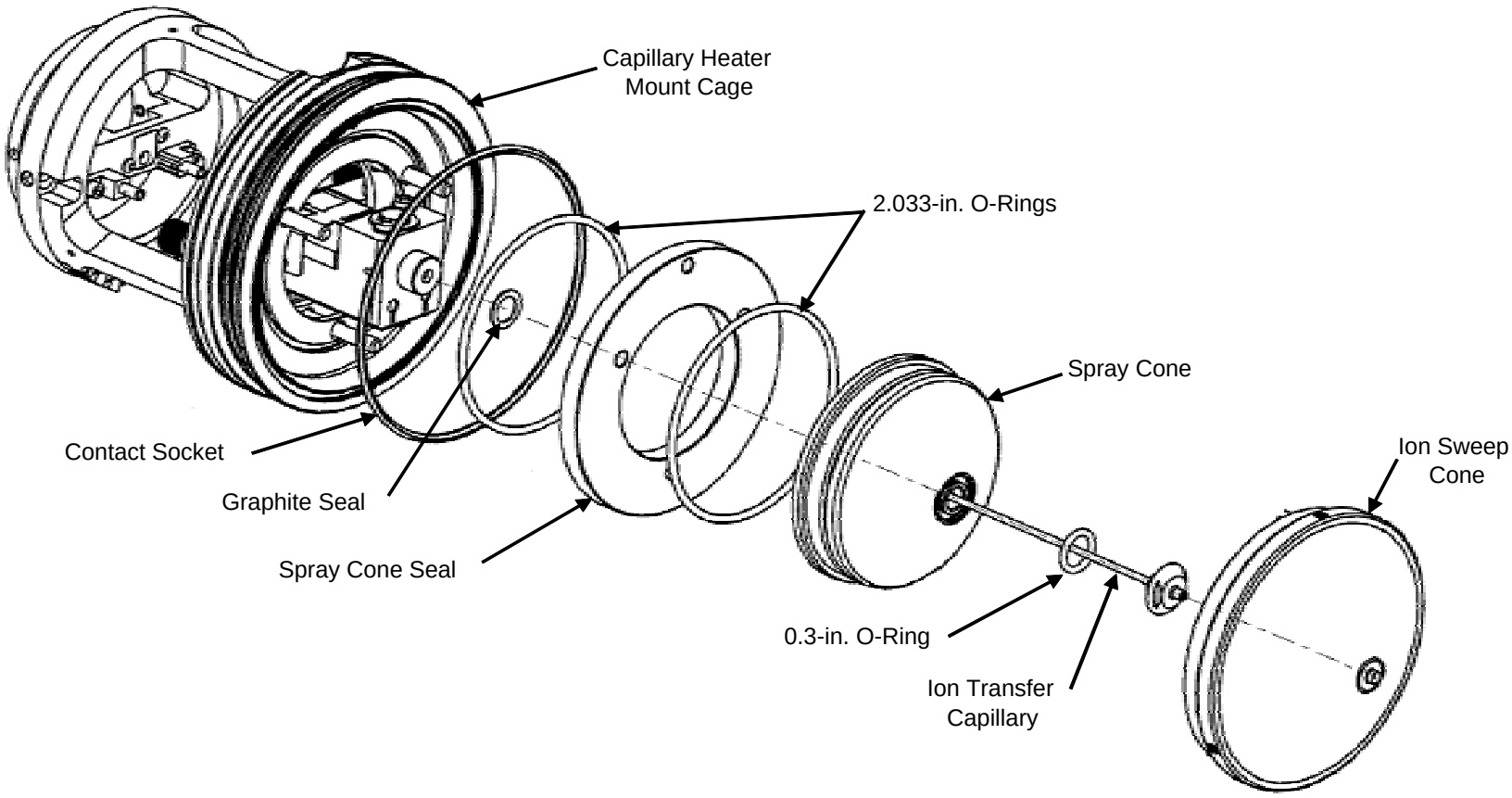


Figure 4-5. Exploded view of the ion source interface (front)

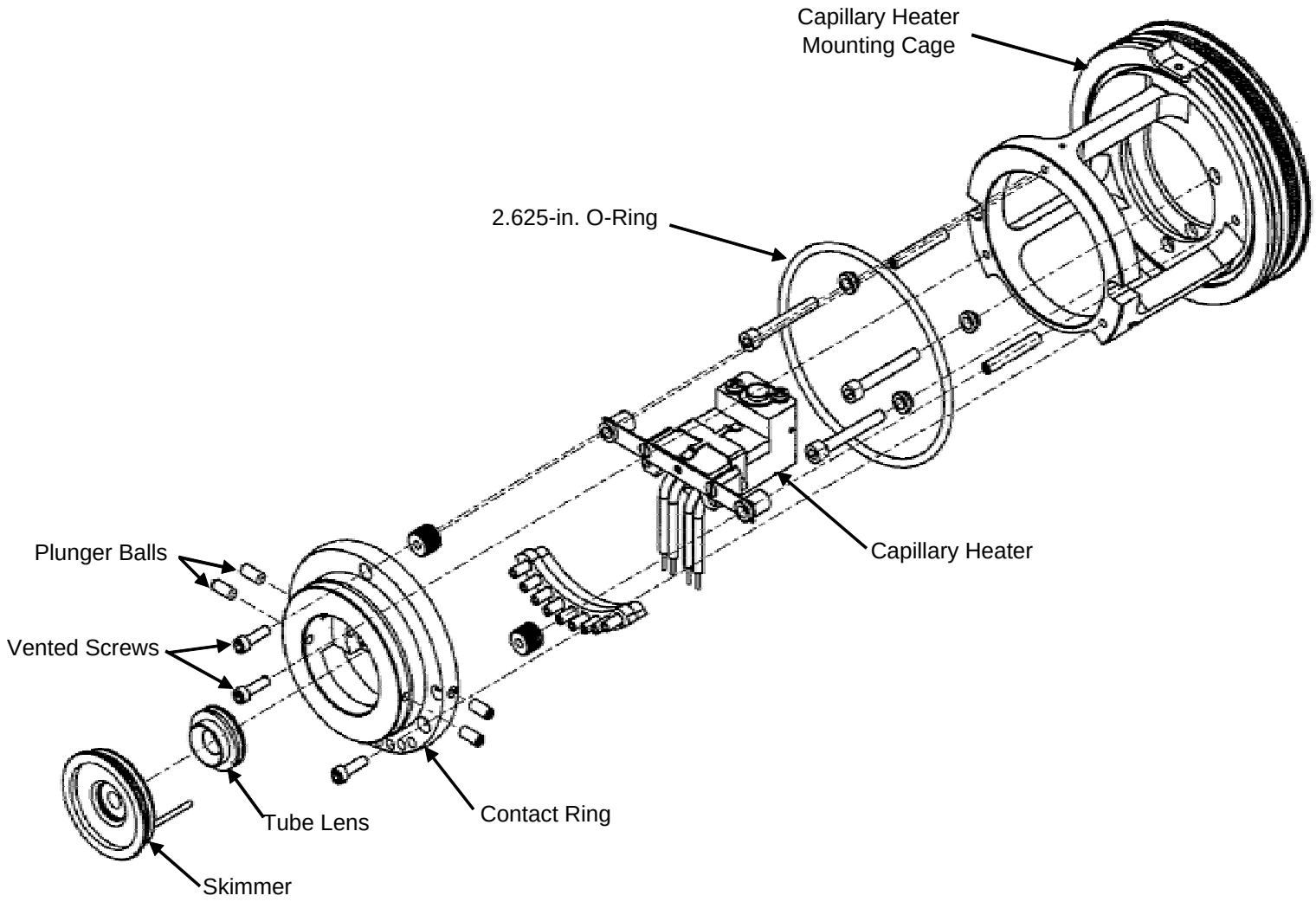


Figure 4-6. Exploded view of the ion source interface (rear)

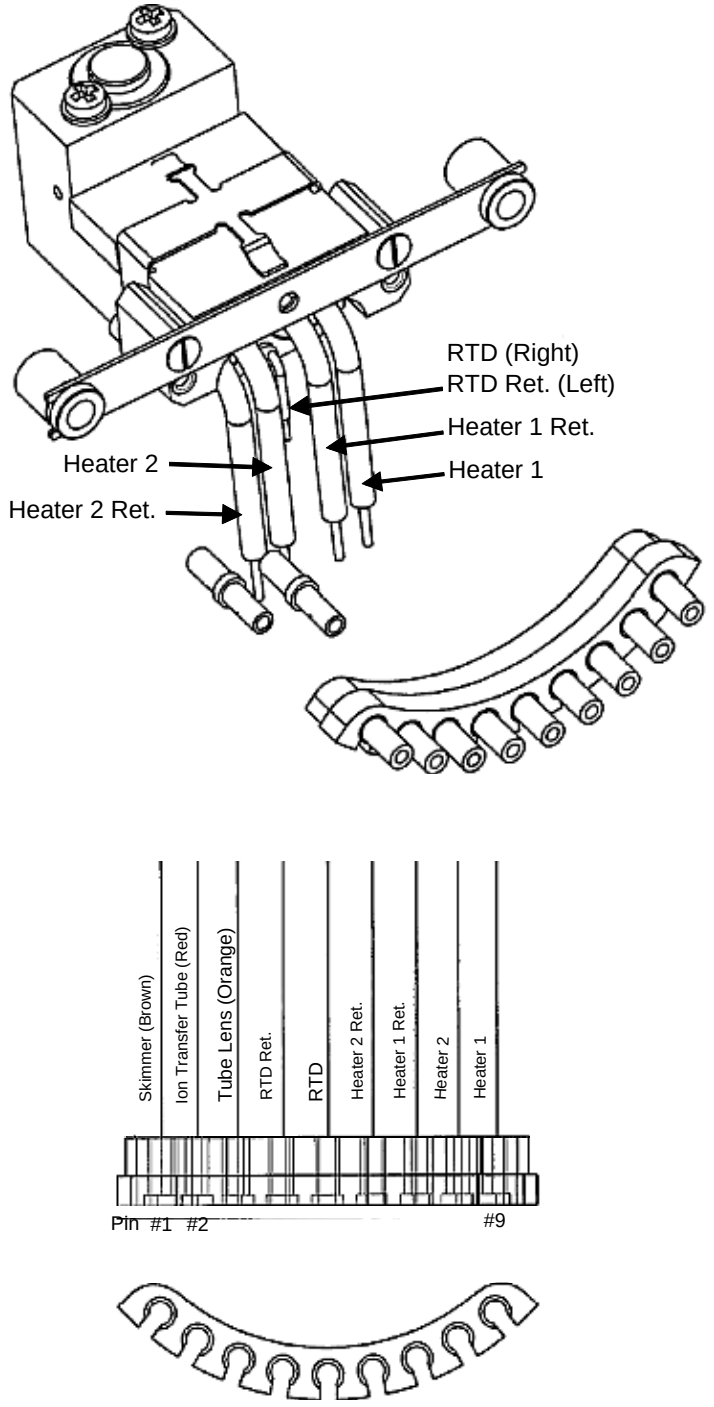


Figure 4-7. Wiring diagram for the ion source interface

Reinstalling the Ion Source Interface

To reinstall the ion source interface proceed as follows:

1. Orient the ion source interface as shown if Figure 4-3.
2. Carefully insert the ion source interface into the vacuum manifold until it seats in the Q00 ion guide.

Go on to the next topic: **Reinstalling the Ion Max Ion Source**.

Reinstalling the Ion Max Ion Source

Reinstall the Ion Max ion source as follows:

1. Carefully align the two guide pin holes on the rear of the source housing with the ion source housing guide pins on the mass spectrometer, and carefully press the ion source housing onto the ion source mount. See Figure 4-8 and Figure 4-9.
   a. Rotate the ion source housing locking levers 90 degrees to lock the ion source housing onto the ion source mount assembly.

> **Caution.** Prevent solvent waste from backing up into the ion source and mass spectrometer. Always ensure that liquid in the drain tube is able to drain to a waste container and that the outlet of the drain tube is above the level of liquid in the waste container.

2. Reinstall the source drain tube as follows:

> **Caution.** Do **not** vent the Ion Max ion source drain tube (or any vent tubing connected to the waste container) to the same fume exhaust system to which you have connected the forepumps. The analyzer optics can become contaminated if the Ion Max ion source drain tube and the (blue) forepump exhaust tubing are connected to the same fume exhaust system.
>
> Your laboratory must be equipped with at least two fume exhaust systems. Route the (blue) forepump exhaust tubing to a dedicated fume exhaust system. Route the drain tube from the Ion Max ion source to a waste container. Vent the waste container to a dedicated fume exhaust system.

   a. Connect the 1-in. ID Tygon tubing (P/N 00301-22922) to the ion source housing drain fitting.
   b. Attach the free end of the hose to a waste container. Ideally, the waste container should be vented to a fume exhaust system.

Go on to the next topic: **Starting Up the System**.

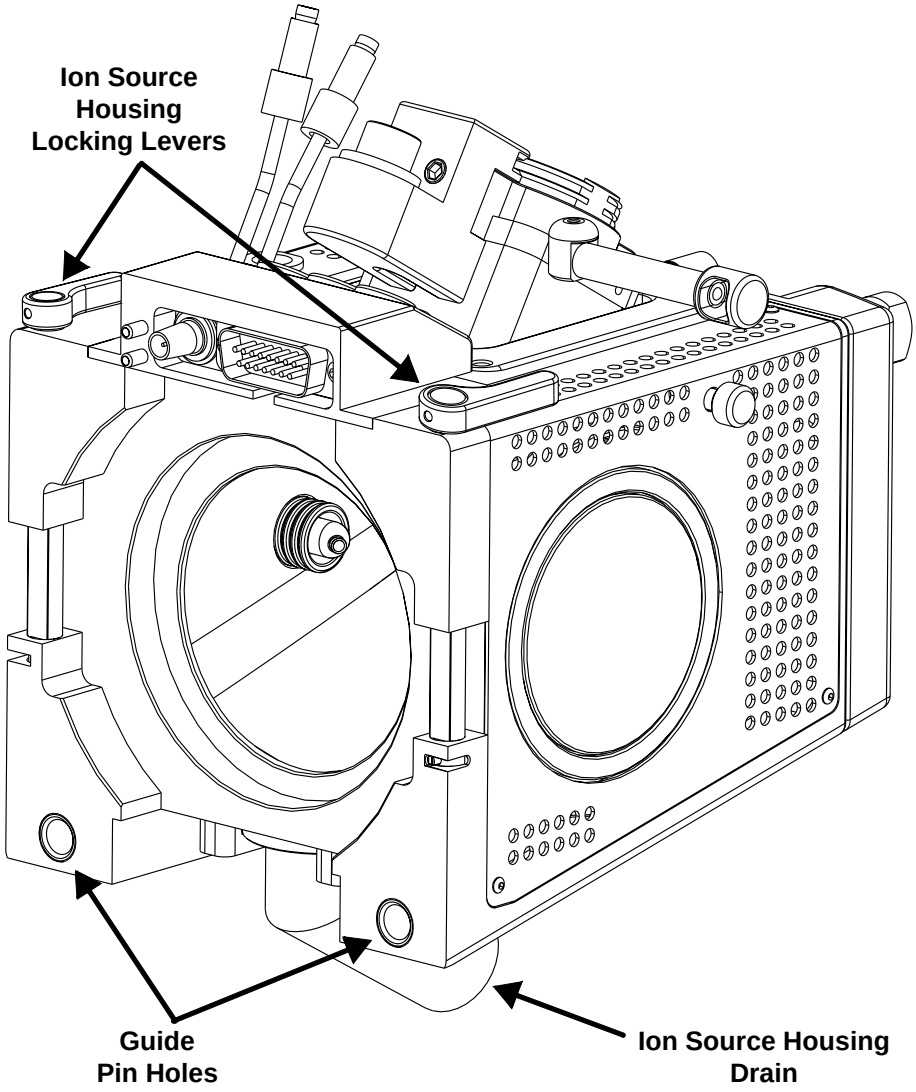


Figure 4-8. Rear view of the Ion Max ion source housing

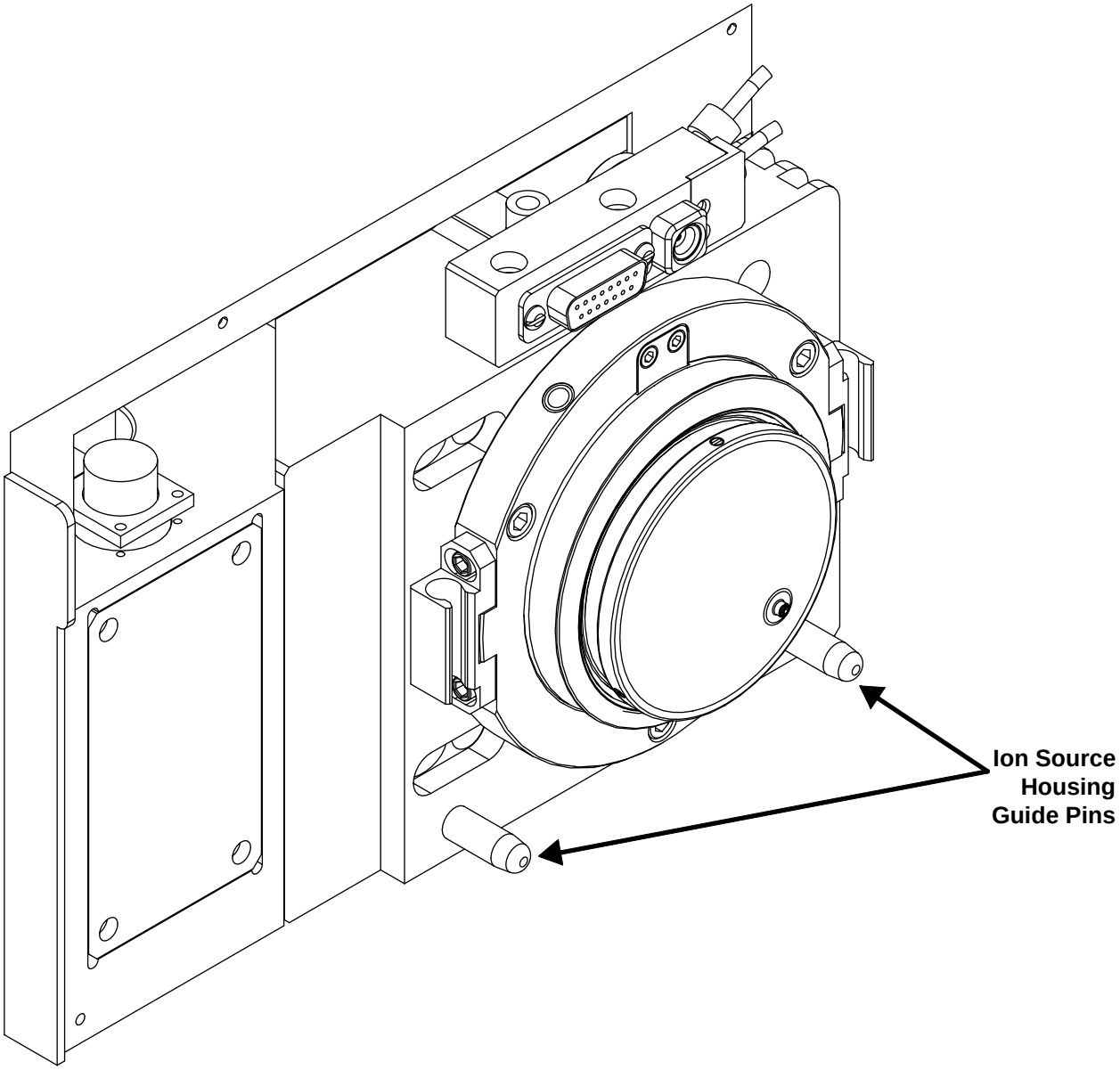


Figure 4-9. Ion source mount showing ion source housing guide pins

Starting Up the System

Start up the system as described in the topic **Starting Up the System After a Complete Shutdown** in the **System Shutdown, Startup, and Reset** chapter.

4.4 Cleaning the Q00 Ion Guide

An accumulation of chemicals on the surfaces of the Q00 quadrupole and lens L0 forms an insulating layer that can modify the electrical fields that control ion transmission. Therefore, clean ion guide components are essential for the proper operation of the instrument. The Q00 quadrupole and lens L0 require cleaning less often than the tube lens and skimmer. The frequency of cleaning depends on the type and quantity of the compounds that you analyze.

To clean or replace the Q00 ion guide components, do the following:

- Shut down and vent the system
- Remove the Ion Max ion source
- Remove the ion source interface
- Remove the Q00 ion guide
- Disassemble the Q00 ion guide
- Clean Q00 quadrupole and lens L0
- Reassemble the Q00 ion guide
- Reinstall Q00 ion guide
- Reinstall the ion source interface
- Reinstall the Ion Max ion source
- Start up the system

Shutting Down the System

Shut down and vent the system as described in the topic **Shutting Down the System Completely** in the **System Shutdown, Startup, and Reset** chapter.

CAUTION. Make sure that the LTQ power cord is unplugged before you proceed.

Go on to the next topic: **Removing the Ion Max Ion Source**.

Removing the Ion Max Ion Source

You need to remove the Ion Max ion source to access the ion source interface and Q00 ion guide. Remove the Ion Max ion source from the front of the MS detector as described in the topic **Removing the Ion Max Ion Source** on page 4-12.

Go on to the next topic: **Removing the Ion Source Interface**.

Removing the Ion Source Interface

You need to remove the ion source interface to access the Q00 ion guide. Remove the ion source interface as described in the topic **Removing the Ion Source Interface** on page 4-13.

Go on to the next topic: **Removing the Q00 Ion Guide**.

Removing the Q00 Ion Guide

To remove the Q00 ion guide, proceed as follows:

1. Reach into the opening in the vacuum manifold (where the ion source interface was) and disconnect the electrical connector to the Q00 ion guide.
2. Loosen the three mounting bolts that hold the Q00 ion guide housing to the vacuum manifold. See Figure 4-10.
3. Carefully remove the Q00 ion guide and place it on a clean surface.

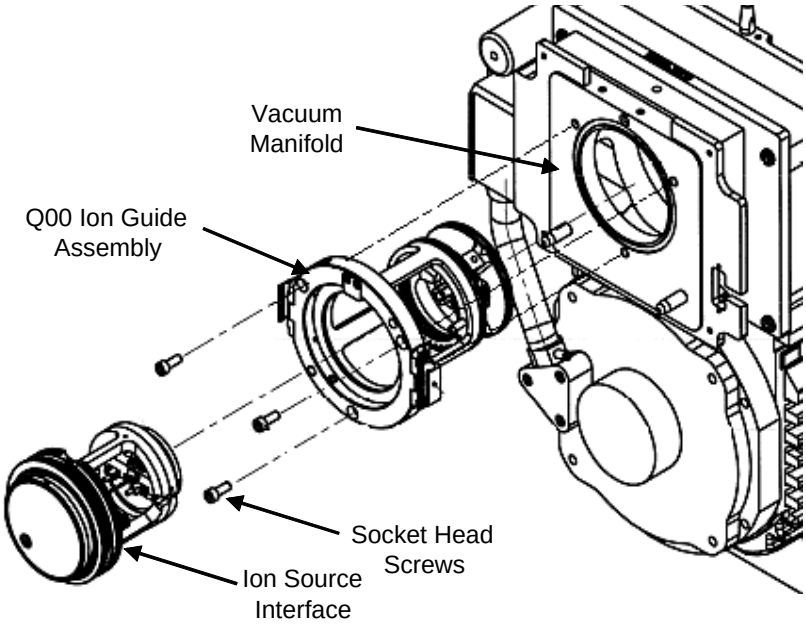


Figure 4-10. Q00 ion guide assembly removal

.Go on to the next topic: **Disassembling the Q00 Ion Guide**.

Disassembling the Q00 Ion Guide

To disassemble the Q00 ion guide, proceed as follows.

> **Note.** Prepare a clean work area by covering the area with lint-free paper. Wear clean gloves when you handle the Q00 ion guide components.

> **Caution.** Be careful not to bend or break the lead pins on the Q00 quadrupole.

1. Carefully remove the leads from the lead pins on the Q00 quadrupole and lens L0. See Figure 4-11.
2. Remove lens L0 from the rear of the Q00 ion guide cage. (Lens L0 is secured to the Q00 ion guide cage by plunger balls.) See Figure 4-12 for the location of the Q00 ion guide components.
3. Remove the Q00 quadrupole from the front of the Q00 ion guide cage. (The Q00 quadrupole is secured to the Q00 ion guide cage by plunger balls.)

Go on to the next topic: **Cleaning the Q00 Ion Guide Components**.

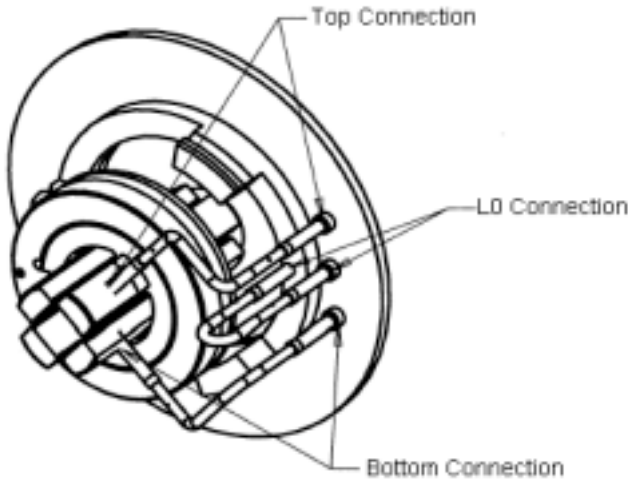


Figure 4-11. Q00 quadrupole and lens L0 wiring

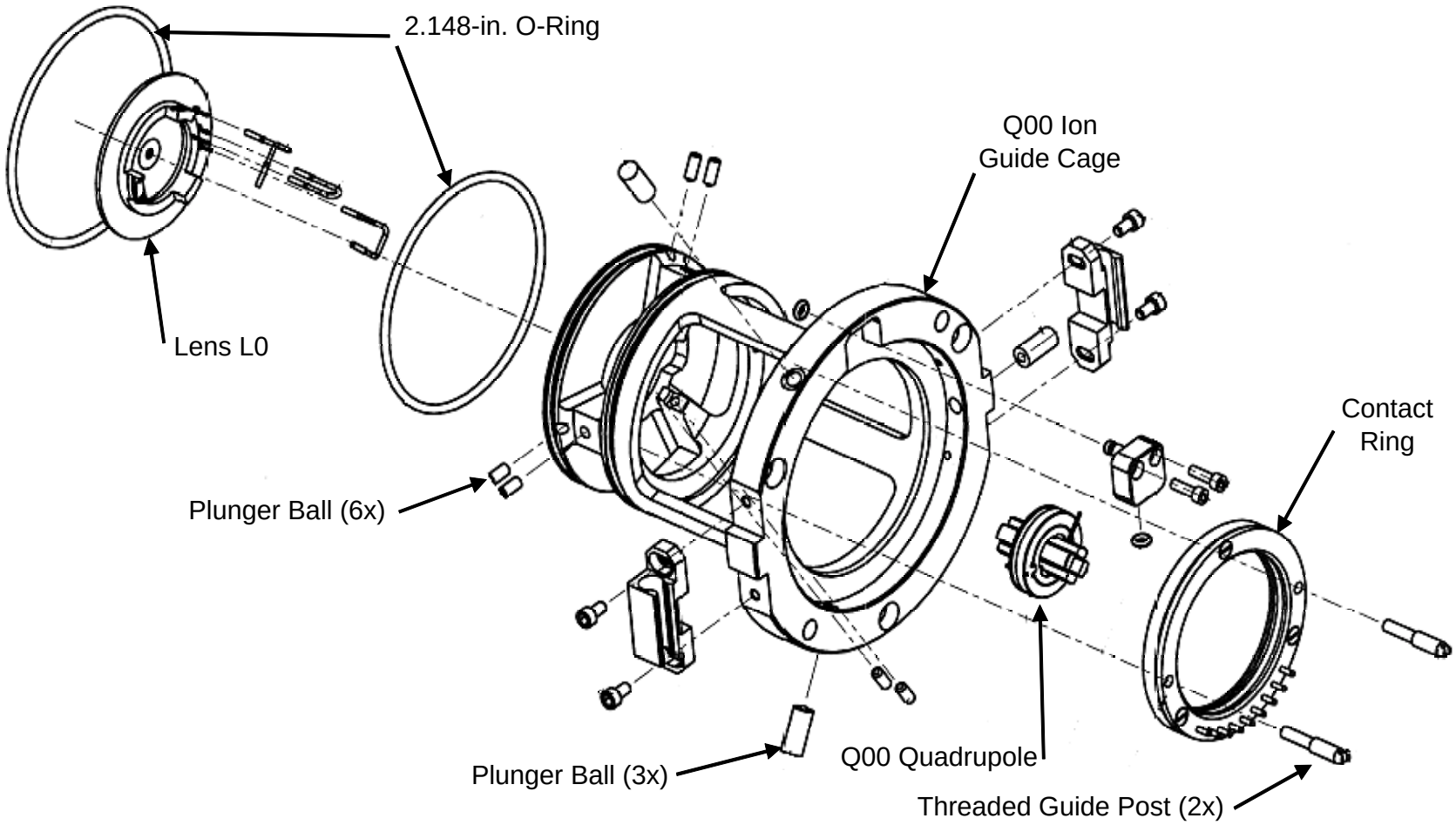


Figure 4-12. Exploded view of the Q00 ion guide

Cleaning the Q00 Ion Guide Components

Use the following procedure to clean the Q00 quadrupole and lens L0.

1. With a soft toothbrush or lint-free swab, scrub the part with a solution of detergent and water.
2. Rinse the part with tap water to remove the detergent.
3. Rinse the part with distilled water.
4. Place the part in a beaker and immerse it completely in HPLC-grade methanol. Move the part up and down in the methanol for 15 s.

> **Note.** Wear clean gloves to handle the parts after you clean them in methanol.

5. Remove the part from the methanol bath; then rinse it thoroughly with fresh methanol.
6. Dry the part with a rapid stream of nitrogen gas.
7. Inspect each part for contamination and dust. If necessary, repeat the cleaning procedure.

Go on to the next topic: **Reassembling the Q00 Ion Guide**.

Reassembling the Q00 Ion Guide

Reassemble the Q00 ion guide as follows:

1. Insert the Q00 quadrupole through the front of the Q00 ion guide cage until it seats in the cage.
2. Insert lens L0 through the rear of the Q00 ion guide cage until it seats in the cage.

> **Caution.** Be careful not to bend or break the lead pins on the Q00 quadrupole.

3. Carefully reconnect the leads to the lead pins on the Q00 quadrupole and lens L0 as shown in Figure 4-11.

Go on to the next topic: **Reinstalling the Q00 Ion Guide**.

Reinstalling the Q00 Ion Guide

Reinstall the Q00 ion guide in the vacuum manifold as follows:

1. Insure that the two 2.148-in. O-rings (P/N 00107-15542) are properly installed on the rear of the Q00 ion guide cage.

2. Orient the Q00 ion guide assembly as shown in Figure 4-10 on page 4-23.
3. Carefully insert the Q00 ion guide assembly into the vacuum manifold.
4. Reconnect the electrical connections.

Go on to the next topic: **Reinstalling the Ion Source Interface**.

Reinstalling the Ion Source Interface

Reinstall the ion source interface as described in the topic **Reinstalling the Ion Source Interface** on page 4-19.

Go on to the next topic: **Reinstalling the Ion Max Ion Source**.

Reinstalling the Ion Max Ion Source

Reinstall the Ion Max ion source as described in the topic **Reinstalling the Ion Max Ion Source** on page 4-19 .

Go on to the next topic: **Starting Up the System**.

Starting Up the System

Start up the system as described in the topic **Starting Up the System After a Complete Shutdown** in the **System Shutdown, Startup, and Reset** chapter.

4.5 Cleaning the Q0 and Q1 Ion Guides

An accumulation of chemicals on the surfaces of the Q0 and Q1 ion guides forms an insulating layer that can modify the electrical fields that control ion transmission. Therefore, clean ion guide components are essential for the proper operation of the instrument. The Q0 and Q1 ion guides require cleaning less frequently than the Q00 ion guide. The frequency of cleaning depends on the type and quantity of the compounds that you analyze.

Cleaning or replacing Q0 and Q1 ion guide components involves the following steps:

- Shut down and vent the system
- Remove the top cover of the MS detector
- Remove the top cover plate of the vacuum manifold
- Remove the Q0 and Q1 ion guides
- Clean the Q0 quadrupole, Q1 octapole, lens L1, and gate lens
- Reinstall the Q0 and Q1 ion guides
- Reinstall the top cover plate of the vacuum manifold
- Reinstall the top cover of the MS detector
- Start up the system

Shutting Down the System

Shut down and vent the system as described in the topic **Shutting Down the System Completely** in the **System Shutdown, Startup, and Reset** chapter.

CAUTION. Make sure that the LTQ power cord is unplugged before you proceed.

Go on to the next topic: **Removing the Top Cover of the MS Detector**.

Removing the Top Cover of the MS Detector

Remove the top cover of the MS detector as follows:

1. Open the front door of the MS detector by loosening the Allen screw on the right side of the door with an Allen wrench.
2. Remove the top cover of the MS detector:
   a. Loosen the two fasteners that hold the top cover to the MS detector chassis. The fasteners are located in the upper right and left corners of the chassis.
   b. Slide the top cover forward by about 1.2 cm (0.5 in.).

c. With one hand under the center of the top cover, lift the top cover up and away from the MS detector.

Go on to the next topic: **Removing the Top Cover Plate of the Vacuum Manifold**.

Removing the Top Cover Plate of the Vacuum Manifold

You need to remove the top cover plate of the vacuum manifold to access the Q0 and Q1 ion guides, mass analyzer, and ion detection system. The top cover plate is held in place by gravity and by the air pressure differential between the vacuum manifold and atmospheric pressure. Six cables are connected to the top cover plate. See Figure 4-12.

To remove the top cover plate, proceed as follows:

1. Disconnect the electron multiplier high voltage coaxial cables that come from the electron multiplier power supply.
2. Disconnect the electrometer cable from the Electrometer PCB. (If necessary, use a small screw driver to loosen the screws that secure the cable.)
3. Disconnect the three cables that connect to the Top Cover PCB.
4. Carefully lift the top cover plate straight up by its two handles. Take care not to damage the components on the underside of the cover plate. Place the cover plate upside down (supported on its handles) on a flat surface.
5. Cover the opening in the top of the vacuum manifold with a large, lint-free tissue.

Go on to the next topic: **Removing the Q0 and Q1 Ion Guides**.

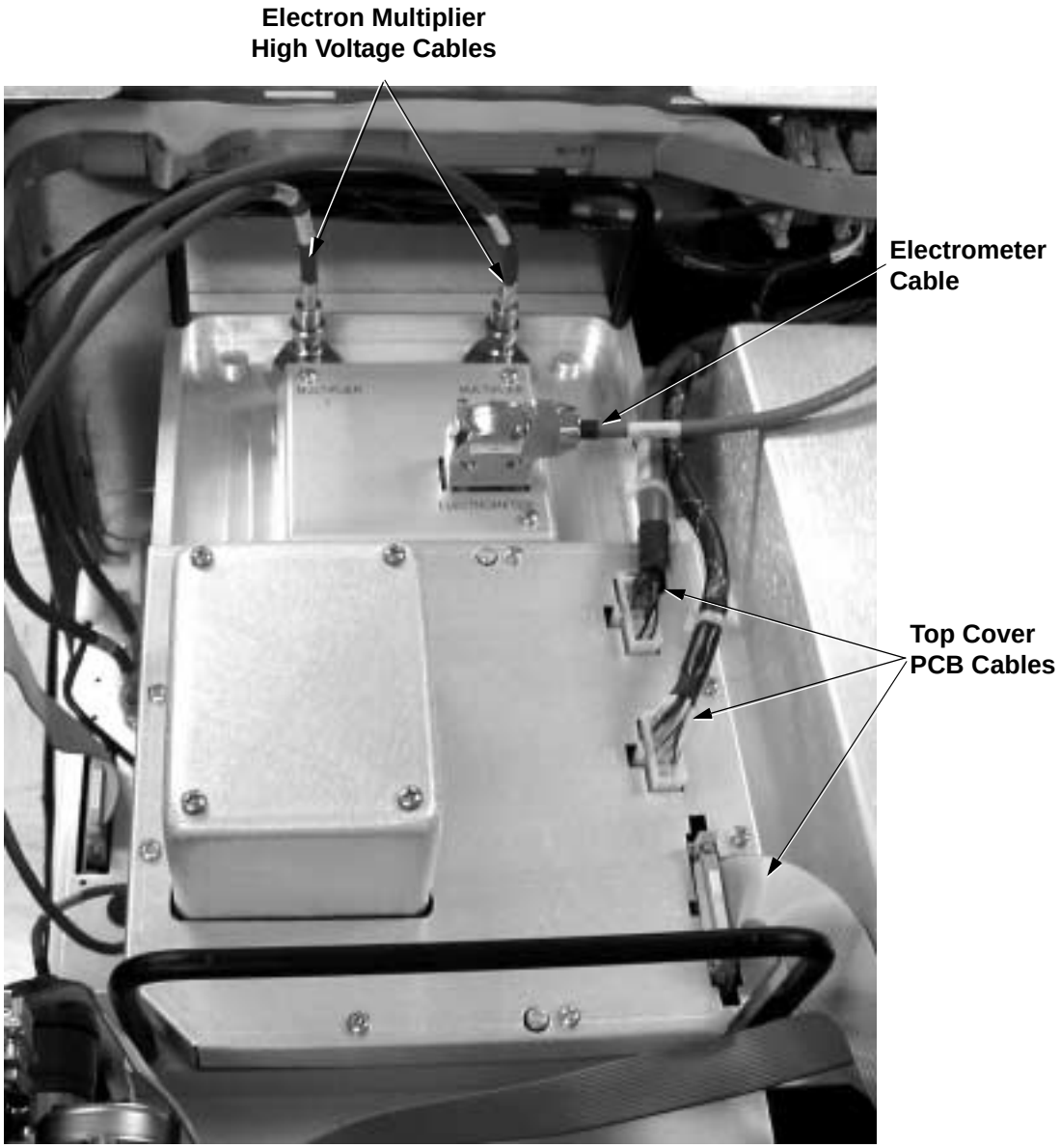


Figure 4-13. Electrical connections to the top cover plate of the vacuum manifold

Removing the Q0 and Q1 Ion Guides

Two adjustable mounting brackets hold the Q0 and Q1 ion guides in position against the baffle on the top cover plate of the vacuum manifold. See Figure 4-14.

Use the following procedure to remove the Q0 and Q1 ion guides from the top cover plate.

> **Note.** Wear clean, lint-free, nylon or cotton gloves when you handle the ion guides.

1. Prepare a clean work area by covering the area with lint-free paper. Place each part on the paper as you remove it.

> **Caution.** Be careful not to bend or break the lead pins on the Q0 quadrupole and Q1 octapole.

2. Disconnect the electrical leads to the Q0 quadrupole, lens L1, gate lens, and Q1 octapole.
3. Hold the Q0 quadrupole and lens L1 with one hand; loosen and remove the two thumb screws that hold the Q0 ion guide mounting bracket to the top cover plate of the vacuum manifold. See Figure 4-14.
4. Remove the Q0 quadrupole and lens L1.
5. Hold the Q1 octapole and gate lens with one hand; loosen and remove the two thumb screws that hold the Q1 ion guide mounting bracket to the top cover plate of the vacuum manifold. See Figure 4-14.
6. Remove the Q1 octapole and gate lens.

Go on to the next topic: **Cleaning the Q0 and Q1 Ion Guides**.

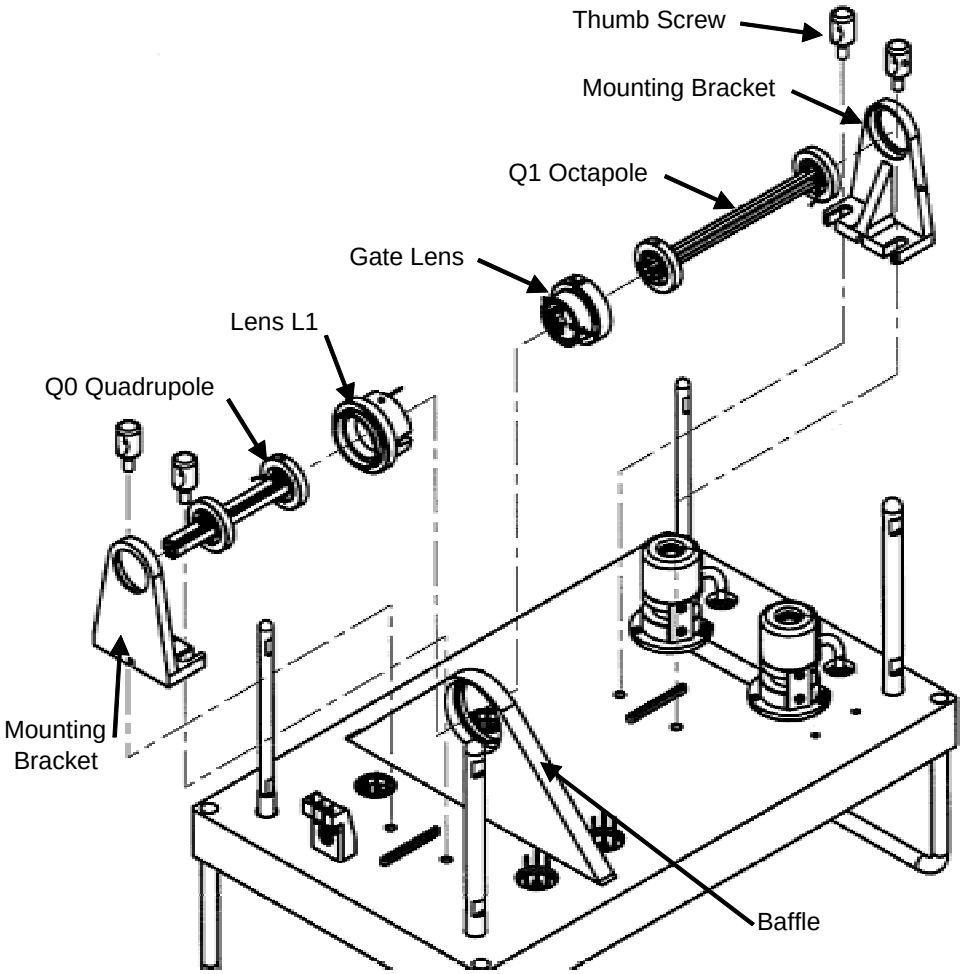


Figure 4-14. Exploded view of the Q0 and Q1 ion guides

Cleaning the Q0 and Q1 Ion Guides

Use the following procedure to remove contamination from the Q0 quadrupole, Q1 octapole, lens L1, and the gate lens. Clean each part in turn. After cleaning, place each part on a clean, lint free surface.

Caution. Take care not to bump or jar the Q0 quadrupole and Q1 octapole.

Note. When you clean the ion guide parts, pay particular attention to the inside surfaces.

1. With a soft tooth brush or lint-free swab, scrub the ion guide part with a solution of detergent and water.
2. Rinse the part with tap water to remove the detergent.
3. Rinse the part with distilled water.
4. Place the part in a tall beaker and immerse it completely in HPLC-grade methanol. Move the part up and down in the methanol for 15 s.

> **Note.** Wear clean, lint-free, nylon or cotton gloves to handle the parts after you clean them in methanol.

5. Remove the part from the methanol bath; then rinse it thoroughly with fresh methanol.
6. Dry the part with a rapid stream of nitrogen gas.
7. Inspect each part for contamination and dust. If necessary, repeat the cleaning procedure.

After all ion optics and mass analyzer parts are clean and dry, go on to the next topic: **Reassembling the Ion Optics and Mass Analyzer**.

Reinstalling the Q0 and Q1 Ion Guides

Two adjustable mounting brackets hold the Q0 and Q1 ion guides in position against the baffle on the top cover plate of the vacuum manifold. See Figure 4-14.

Use the following procedure to reinstall the Q0 and Q1 ion guides on the top cover plate.

> **Note.** Wear clean, lint-free, nylon or cotton gloves when you handle the ion guides.

1. Install the Q1 ion guide as follows:
   a. Insert the gate lens into the opening in the baffle (Figure 4-14).
   b. With one hand, hold the Q1 octapole against the gate lens; with the other hand, install the Q1 ion guide mounting bracket so that the octapole is held between the mounting bracket and the gate lens.
   c. Tighten the two thumb screws that hold the Q1 ion guide mounting bracket to the top cover plate.

2. Install the Q0 ion guide as follows:
   a. Insert lens L1 into the opening in the baffle (Figure 4-14).
   b. With one hand, hold the Q0 quadrupole against the lens L1; with the other hand, install the Q0 ion guide mounting bracket so that the quadrupole is held between the mounting bracket and the lens L1.
   c. Tighten the two thumb screws that hold the Q0 ion guide mounting bracket to the top cover plate.

> **Caution.** Be careful not to bend or break the lead pins on the Q0 quadrupole and Q1 octapole.

3. Reconnect the electrical leads to the Q0 quadrupole, lens L1, gate lens, and Q1 octapole according to the wiring diagram shown in Figure 4-15.

> **Note**. Check all leads and ensure that they are secure and that they go to the proper electrodes.

Go on to the next topic: **Cleaning the Ion Detection System**.

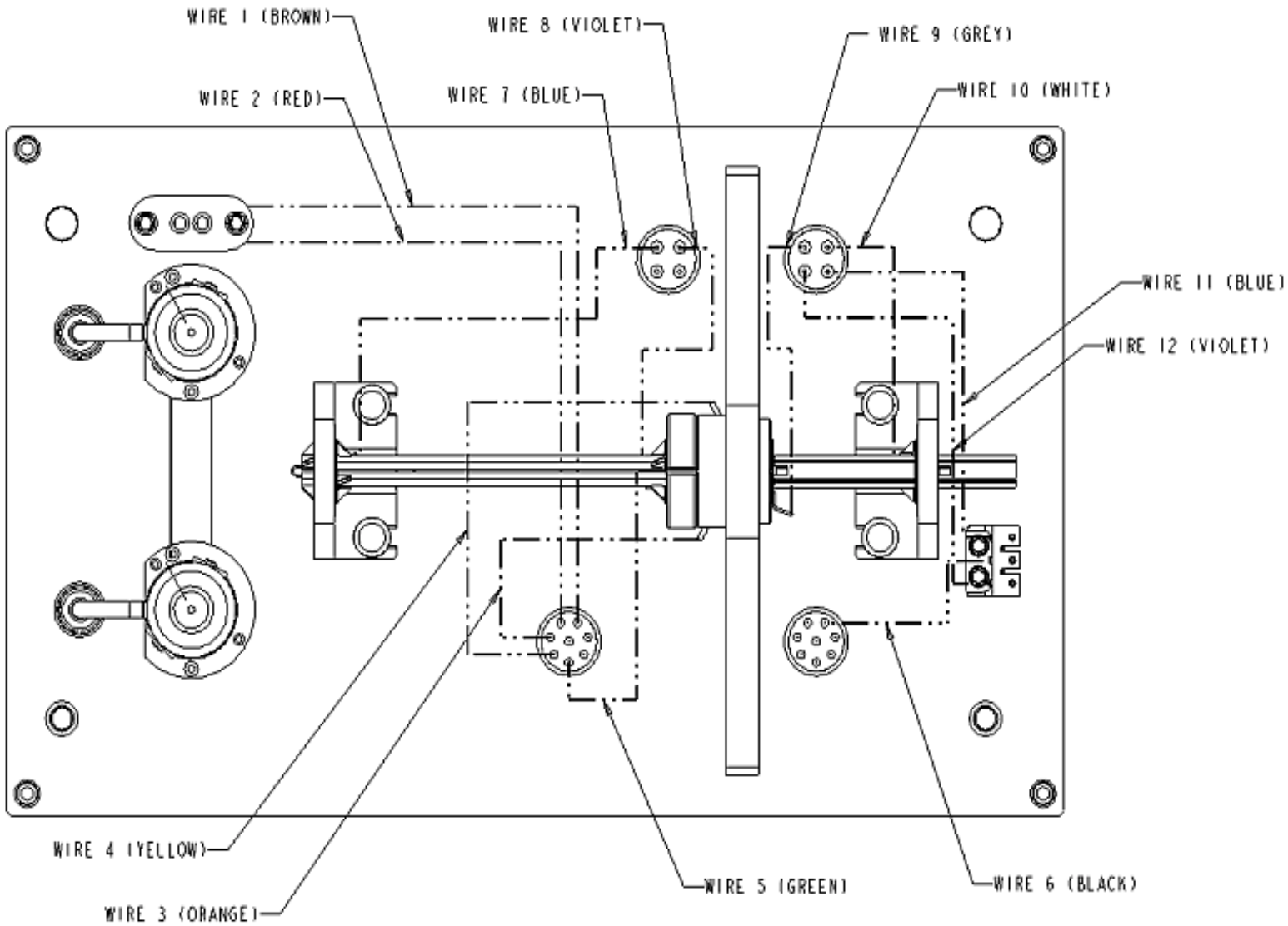


Figure 4-15. Wiring diagram for the Q0 and Q1 ion guides

Cleaning the Ion Detection System

The conversion dynode and electron multiplier of the ion detection system must be kept dust free. Clean the conversion dynodes and electron multipliers whenever you remove the top cover plate of the vacuum manifold. Cleaning the conversion dynodes and electron multipliers involves only blowing them with clean, dry gas such as nitrogen. Freon gas is not recommended. **Do not use liquids to clean the ion detection system components.** 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.

Go on to the next topic: **Reinstalling the Top Cover Plate of the Vacuum Manifold**.

Reinstalling the Top Cover Plate of the Vacuum Manifold

Use the following procedure to reinstall the top cover plate of the vacuum manifold:

1. Remove the tissue from the opening in the top of the vacuum manifold.
2. Check the O-ring that surrounds the opening for signs of wear, and replace it if necessary (P/N 97055-40005). Make sure that the O-ring is seated properly.

> **Note.** Periodically, remove any contamination that might be on the inner walls of the manifold by wiping the inner walls with a lint-free tissue soaked in HPLC-grade methanol. Use a cotton-tipped applicator soaked in methanol to clean around inlets and feedthroughs.

3. Carefully lift the top cover plate up by its two handles and turn it over. Orient the top cover plate such that the electron multiplier is over the conversion dynode. Carefully insert the guide posts on the underside of the top cover plate into the guide holes in the vacuum manifold. Slowly lower the cover plate onto the opening in the vacuum manifold. Take care not to damage the components on the underside of the cover plate. Ensure that the cover plate is seated properly on the vacuum manifold.
4. Reconnect the three cables to the Top Cover PCB. See figure 4-14 on page 4-31.
5. Reconnect the electron multiplier high voltage coaxial cables that come from the electron multiplier power supply.
6. Reconnect the electrometer cable to the Electrometer PCB.

Go on to the next topic: **Reinstalling the Top Cover of the MS Detector**.

Reinstalling the Top Cover of the MS Detector

Reinstall the top cover of the MS detector as follows:

1. Open the front door of the MS detector by loosening the Allen screw on the right side of the door with an Allen wrench or hex-head ball driver.
2. With one hand under the center of the top cover, place the top cover over the MS detector such that the front of the cover is about 1.2 cm (0.5 in.) in front of the front of the MS detector.
3. Slide the cover back until it is flush with the front doors (when they are closed).
4. Tighten the two fasteners to secure the top cover to the chassis.
5. Close the front door of MS detector. Tighten the Allen screw on the right side of the door with an Allen wrench or hex-head ball driver.
6. Reconnect any tubing between the syringe pump and the API source to accommodate your instrument configuration.

Go on to the next topic: **Starting Up the System**.

Starting Up the System

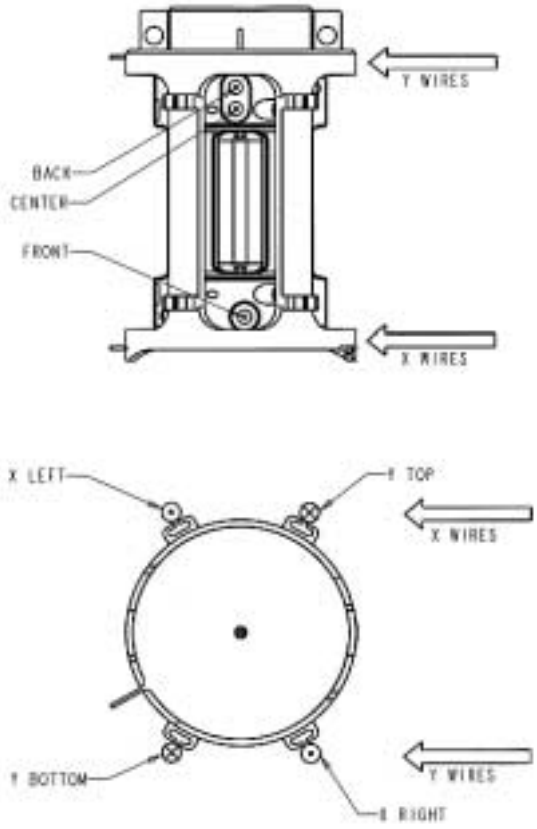
Start up the system as described in the topic **Starting Up the System After a Complete Shutdown** in the **System Shutdown, Startup, and Reset** chapter.

4.6 Mass Analyzer Maintenance

The mass analyzer requires cleaning very rarely, if ever.

> **Caution.** The hyperbolic rods of the mass analyzer are precision-aligned at the factory. Due to the delicate nature of the mass analyzer, mass analyzer maintenance should be performed only by a Thermo Electron Field Service Engineer.

A wiring diagram for the mass analyzer is shown in Figure 4-16.



WIRE CONNECTIONS

CONNECTOR	PIN	COLOR	ROD	SEGMENT
X (TOP)	1	RED	LEFT	BACK
X (TOP)	2	BRN	LEFT	CENTER
X (TOP)	3	BLK	LEFT	FRONT
X (TOP)	4	ORG	RIGHT	FRONT
X (TOP)	5	YEL	RIGHT	CENTER
X (TOP)	6	GRN	RIGHT	BACK
Y (BOT)	1	GRY	TOP	BACK
Y (BOT)	2	VIO	TOP	CENTER
Y (BOT)	3	BLU	TOP	FRONT
Y (BOT)	4	BLU	BOTTOM	FRONT
Y (BOT)	5	VIO	BOTTOM	CENTER
Y (BOT)	6	GRY	BOTTOM	BACK

Figure 4-16. Wiring diagram for the mass analyzer

4.7 Replacing the Electron Multiplier

The electron multiplier of the ion detection system includes an anode and a cathode. The anode and cathode have finite lifetimes. The anode loses sensitivity over time due to contamination of its surface. Things that decrease the lifetime of the cathode are: heat; electron flow (which produces internal heat); air (which causes oxidation and arcing); and water (which causes arcing).

The following symptoms suggest that the electron multiplier may need replacing:

- Excessive noise in the mass spectrum
- Inability of the multiplier gain calibration procedure to achieve a gain of 3×10^5 electrons per ion with an electron multiplier voltage less than or equal to 2.5 kV

You can read the current value of the electron multiplier voltage in the Ion Detection System dialog box, which can be reached from the Tune Plus window by choosing **Setup > Ion Detection System**.

If you are having problems with the ion detection system, you need to replace the electron multiplier assembly.

To replace the electron multiplier assembly, proceed as follows:

1. Shut down and vent the system as described in the topic **Shutting the System Down Completely** in the **System Shutdown, Startup, and Reset** chapter.

CAUTION. Make sure that the LTQ power cord is unplugged before you proceed.

2. Remove the top cover of the MS detector as described in the topic **Removing the Top Cover of the MS Detector** on page 4-28.
3. Remove the top cover plate of the vacuum manifold as described in the topic **Removing the Top Cover Plate of the Vacuum Manifold** on page 4-29.

Note. Wear clean, lint-free, nylon or cotton gloves when you handle the electron multiplier components.

4. With an Allen wrench, remove the two socket-head screws that hold the electron multiplier support to the top cover plate of the vacuum manifold. See Figure 4-17.
5. With one hand hold the high voltage tube and with the other hand hold the electron multiplier support. Then, detach the high voltage tube from the

high voltage feedthrough in the top cover plate and remove the electron multiplier as a unit. (The anode remains in the anode feedthrough in the top cover plate.)

6. Repeat steps 4 and 5 with the second electron multiplier.
7. Remove the anode shield (Figure 4-17).
8. Loosen the socket-head screw that secures the dual anode. Remove the dual anode from the anode feedthrough.
9. Install a new dual anode (P/N 97055-20018) in the anode feedthrough in the top cover plate. Secure the dual anode with the socket-head screw.
10. Reinstall the anode shield over the dual anode.

> **Caution.** Be careful not to damage the surface of the electron multiplier shield. The electron multiplier shield has been electropolished to prevent field emission.

11. With one hand holding the high voltage tube and the other hand holding the electron multiplier support, install the new electron multiplier (P/N 96000-60036) on the top cover plate. Ensure that the high voltage tube is properly inserted in the high voltage feedthrough and that the screw holes in the electron multiplier support are aligned with the screw holes in the top cover plate.

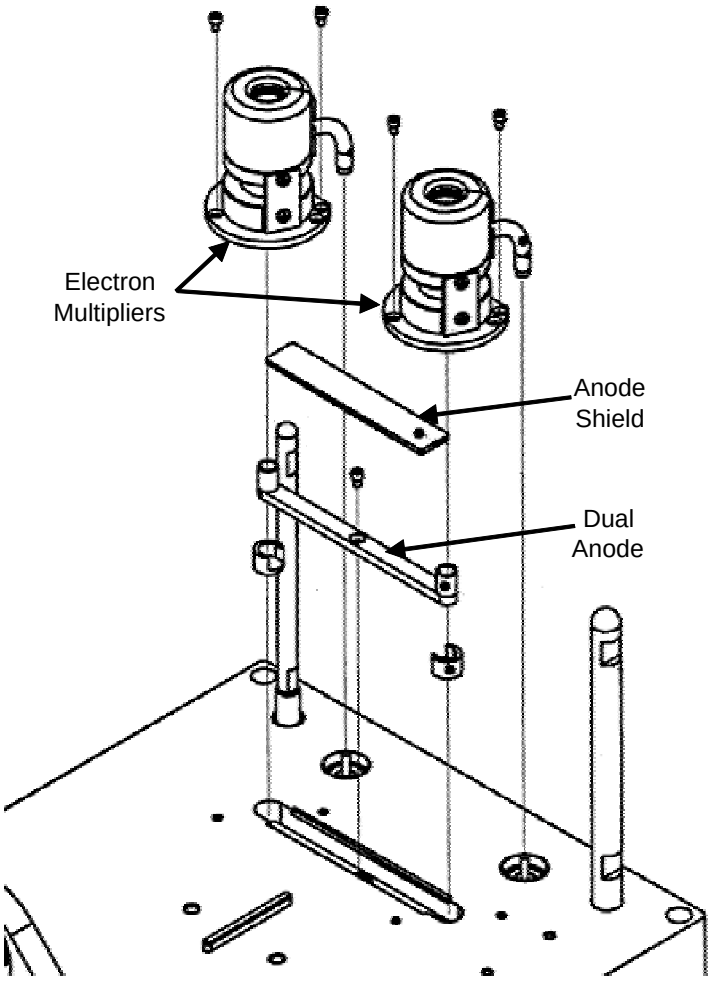


Figure 4-17. Electron multipliers and dual anode

12. Reinstall the two socket-head screws that secure the electron multiplier support to the top cover plate. Tighten the screws with an Allen wrench.
13. Repeat steps 11 and 12 with the second electron multiplier.
14. Reinstall the top cover plate of the vacuum manifold over the opening in the vacuum manifold as described in the topic **Reinstalling the Top Cover Plate of the Vacuum Manifold** on **Reinstalling the Top Cover Plate of the Vacuum Manifold** on page 4-36.
15. Reinstall the top cover of the MS detector as described in the topic **Reinstalling the Top Cover of the MS Detector** on page 4-37.
16. Start up the LTQ system as described in the topic **Starting Up the System After a Complete Shutdown in the System Shutdown, Startup, and Reset** chapter.
17. Set the electron multiplier voltage to -800 V as follows:

a. Choose **Start > Programs > Xcalibur > LTQ Tune** to open the Tune Plus window.

b. From the Tune Plus window, choose **Diagnostics > Diagnostics**.

c. Select (General) Graphs to display the Graphs page.

d. In the Set Device Value option box, select Multiplier 1 (V) or Multiplier 2 (V).

e. In the text box to the right of the Set Device Value option box, enter **-800**.

f. Click on the **Set** button to set the electron multiplier voltage to -800 V.

g. Click on the **OK** button to return to Tune Plus.

18. Calibrate the electron multiplier voltage as follows:

    a. Allow the system to pump down for at least one hour before you turn on the high voltages.

    b. Set up for the infusion of the tuning solution into the MS detector as described in **LTQ Getting Started**.

    c. From the Tune Plus window, choose **Control > Calibrate**. The Calibrate dialog box appears.

    d. Click on the Semi-Automatic tab to display the Semi-Automatic page.

    e. Select the Electron Multiplier Gain option. Click on the **Start** button to start the multiplier gain procedure.

19. After the Electron Multiplier Gain program is finished, set up for operation as described in **LTQ Getting Started**.

4.8 Replacing the Turbomolecular Pump Insert

The rotating, interior portion of the turbomolecular pump, referred to as the turbomolecular pump *insert*, should be replaced after 20,000 to 30,000 hours of operation or if the bearings fail.

Replacing the turbomolecular pump insert involves the following steps:

1. Shutting down the system
2. Removing the left front panel
3. Disconnecting the power cable from the turbomolecular pump
4. Disconnecting the foreline from the turbomolecular pump
5. Loosening and removing the six 4 mm socket-head screws that hold the insert to the pump
6. Removing the insert
7. Reinstalling a new inset
8. Installing and tightening the six screws that hold the insert to the pump
9. Connecting the foreline to the turbomolecular pump
10. Connecting the power cable to the turbomolecular pump
11. Reinstalling the left front panel
12. Starting up the system

> **Caution.** The turbomolecular pump insert is very delicate. We recommend that a Thermo Electron Field Service Engineer replace the turbomolecular pump insert.

4.9 Cleaning the Fan Filter

You need to clean the fan filter (P/N 97055-20254) very four months. The fan filters is located on the rear of the MS detector on the right side. To clean the fan filters, proceed as follows:

1. Remove the fan filter from the rear of the MS detector by pulling it up and out of the fan filter bracket.
2. Wash the fan filters in a solution of soap and water.
3. Rinse the fan filters with tap water.
4. Squeeze the water from the fan filters and allow them to air dry.
5. Reinstall the fan filter in the fan filter bracket.

Chapter 5
System Shutdown, Startup, and Reset

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

In this chapter procedures are provided to do the following:

- Shut down the system in an emergency
- Place the system in standby condition
- Shut down the system completely
- Start up the system after a complete shutdown
- Reset the MS detector
- Reset the tune and calibration parameters to their default values
- Reset the data system
- Turn off selected MS detector components

5.1 Shutting Down the System in an Emergency

If you need to turn off the MS detector in an emergency, place the main power circuit breaker switch, located on the power panel on the right side panel of the MS detector (see Figure 5-1), in the Off (O) position. This turns off all power to the MS detector, including the vacuum pumps. Although removing power abruptly will not harm any component within the system, this is not the recommended shutdown procedure to follow. Refer to the **Shutting Down the System Completely** topic, on page 5-4, for the recommended procedure.

To turn off the LC, autosampler, and computer in an emergency, use the on/off switches on the LC, autosampler, and computer, respectively.

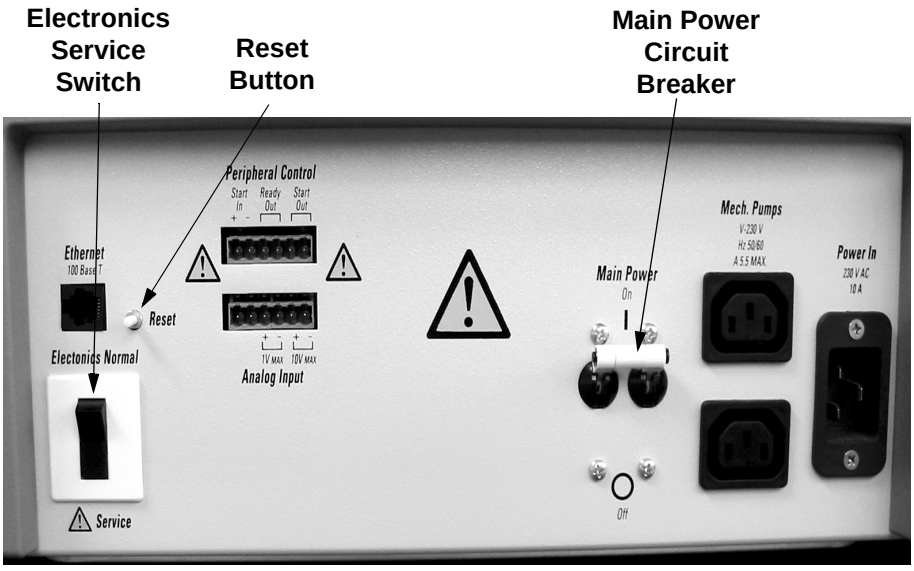


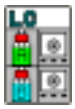
Figure 5-1. Power panel, showing the Reset button electronics service switch, and the main power circuit breaker switch

5.2 Placing the System in Standby Condition

The LTQ 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 weekends. When you are not going to operate the system for 12 hours or more, you can leave the system in a standby condition.

Use the following procedure to place the LTQ 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 to the API source, as follows:



   a. In the Tune Plus window, click on the LC button. The Inlet Direct Control dialog box appears.

   b. Click on  (or **Pump Off** or **Stop Pump)** to stop the LC pump.

> **Caution**. **If you are using APPI:** Do not leave the LC or other liquid delivery device on while the mass spectrometer is in Standby. The absence of sheath and auxiliary gas can cause the hot VUV lamp to break upon contact with liquids.


On


Standby

3. From the Tune Plus window, choose **Control > Standby** (or click on the On/Standby button to toggle it to Standby) to put the MS detector in Standby. When you choose Control > Standby, the LTQ turns off the electron multipliers, conversion dynodes, 8 kV power to the API source, main RF voltage, and ion guide RF voltages. LTQ also turns off the auxiliary and sheath gas flows. See Table 5-1 on page 5-14 for the On/Off status of MS detector components when the MS detector is in the standby condition. The System LED on the front panel of the MS detector is illuminated yellow when the system is in Standby.
4. Flush the spray shield and the entrance end of the ion transfer capillary of the API source as describe in the topic **Flushing the Spray Shield and Ion Transfer Capillary** in the **MS Detector Maintenance** chapter. Cap the ion transfer capillary with the septum. Leave the API flange withdrawn from the spray shield.
5. Purge the rotary-vane pump oil as described in the topic **Purging the Rotary-Vane Pump Oil** in the **MS Detector Maintenance** chapter.
6. Leave the MS detector power on.
7. Leave the LC power on.
8. Leave the autosampler power on.
9. Leave the data system power on.

5.3 Shutting Down the System Completely

The LTQ 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 weekends. (Refer to the topic **Placing the System in Standby Condition**, above.) Shut down the system completely only if it is to be unused for an extended period or if it must be shut down for a maintenance or service procedure.

Use the following procedure to shut down the LTQ system completely:

1. 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.

2. From the Tune Plus window, choose **Control > Standby** (or click on the On/Standby button) to put the MS detector in Standby. When you place the MS detector in Standby mode, LTQ turns off the electron multiplier, conversion dynode, 8 kV power to the API source, main RF voltage, and octapole RF voltage, sheath and auxiliary gasses.
3. Place the electronics service switch, located on the power panel (see Figure 5-1 on page 5-2), in the Service position. Power to the non-vacuum system electronics is turned off when you place the electronics service switch in the Service position.
4. Place the main power circuit breaker switch, located on the power panel (Figure 5-1) in the Off (O) position. When you place the main power circuit breaker switch in the Off (O) position, the following occurs:
   - All power to the MS detector, including the turbomolecular pump and rotary vane pump, is turned off. (All LEDs on the front panel of the MS detector are off.)
   - The battery backup on the Vent Delay PCB provides power to the vent valve for 30 s. After 30 s, a circuit on the Vent Delay PCB times out, and power to the vent valve solenoid is shut off. When power to the vent valve solenoid is shut off, the vent valve opens and the vacuum manifold is vented to filtered air. You can hear a hissing sound as the air passes through the air filter.
   - After about 2 min, the vacuum manifold is at atmospheric pressure.
5. Unplug the power cord for the MS detector.

> **CAUTION.** Allow heated components to cool before servicing them.

Note. If you are planning to perform routine or preventive system maintenance on the MS detector only, you do not need to turn off the LC, data system, and autosampler. In this case, the shutdown procedure is completed. However, if you do not plan to operate your system for an extended period of time, we recommend that you turn off the LC, data system, and autosampler as described in steps 6 through 11 below.

6. Turn off the (optional) LC. Follow the procedure described in the manual that came with the LC.
7. Turn off the helium damping gas supply at the tank.
8. Turn off the nitrogen supply at the tank.
9. Turn off the data system as follows:
    a. Choose **Start > Shut Down** from the Windows XP task bar. The Shut Down Windows dialog box appears.
    a. Select the Shut Down The Computer option button, and then click on **Yes** to start the Windows XP shutdown procedure.
    b. When the Windows XP shutdown procedure tells you that it is safe to turn off the computer, turn off the monitor and computer by using the on/off switches.
10. Turn off the (optional) printer by using the on/off switch.
11. Turn off the (optional) autosampler by using the main power on/off switch.

5.4 Starting Up the System after a Complete Shutdown

To start up the LTQ system after it has been shut down completely, you need to do the following:

- Start up the (optional) LC
- Start up the data system
- Start up the MS detector
- Start up the (optional) autosampler
- Set up conditions for operation

Starting Up the LC

To start up the LC, follow the startup procedure described in the manual that came with the LC. If necessary, configure the LC as described in **LTQ Getting Connected**. Do not turn on the liquid flow to the MS detector.

Starting Up the Data System

Use the following procedure to start up the data system:

1. Turn on the monitor, computer, and printer.
2. Observe the Windows XP startup procedure on the monitor.
3. Press **<Ctrl>-<Alt>-<Del>** when you are prompted to do so. Then, click on **OK** or enter your password (if you have one) in the Logon Information dialog box to complete the start up procedure.

Starting Up the MS Detector

Use the following procedure to start up the MS detector.

> **Note.** The data system must be running before you start up the MS detector. The MS detector will not operate until software is received from the data system.

1. Turn on the flows of helium and nitrogen at the tanks if they are off.
2. Make sure that the main power circuit breaker switch is in the Off (O) position and the electronics service switch is in the Service position.
3. Plug in the power cord for the MS detector.

4. Place the main power circuit breaker switch in the On (|) position. When you place the main power circuit breaker switch in the On (|) position, the rotary-vane pump and the turbomolecular pump are started. All LEDs on the MS detector front panel are off.
5. Allow the LTQ to pump down for 5 min.
6. Place the electronics service switch in the Electronics Normal position. When you place the electronics service switch in the Electronics Normal position, the following occurs:
   - The Power LED on the MS detector front panel is illuminated green to indicate that power is provided to the MS detector electronics. (The electron multiplier, conversion dynode, 8 kV power to the API source, main RF voltage, and octapole RF voltage remain off.)
   - The embedded computer reboots. After several seconds the Communication LED on the front panel is illuminated yellow to indicate that the data system and the MS detector have started to establish a communication link.
   - After several more seconds, the Communication LED is illuminated green to indicate that the data system and the MS detector have established a communication link. Ensure that the instrument console window is active. Software for the operation of the MS detector is then transferred from the data system to the MS detector.
   - After 3 minutes, the System LED is illuminated yellow to indicate that the software transfer from the data system to the MS detector is complete and that the instrument is in Standby.

Note. The Vacuum LED on the front panel of the MS detector 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).

If you have an autosampler, go on to the next topic: **Starting Up the Autosampler**. If you do not have an autosampler, go to the topic: **Setting Up Conditions for Operation**.

Starting Up the Autosampler

To start up the autosampler, place the main power switch on the autosampler in the on position. If necessary, configure the autosampler. For procedures for placing sample vials, preparing solvent and waste bottles, installing syringes, etc., refer to the manual that came with the autosampler. Refer also to **LTQ Getting Connected**.

Setting Up Conditions for Operation

You need to do the following to set up your LTQ for operation:

1. Before you begin data acquisition with your LTQ system, you need to allow the system to pump down for at least 1 hour. Operation of the system with excessive air and water in the vacuum manifold can cause reduced sensitivity, tuning problems, and reduced lifetime of the electron multiplier.
2. Ensure that the helium pressure and nitrogen pressure are within the operational limits (helium: 40 ±10 psig [275 ±70 kPa], nitrogen: 100 ±20 psig [690 ±140 kPa]).

> **Note.** Air in the helium line must be purged or given sufficient time to be purged for normal LTQ performance.

3. Look at the status panel in the Tune Plus window. Check to see if the pressure measured by the ion gauge is below about 5×10^{-5} Torr, and the pressure measured by the Convectron gauge is around 1 Torr. Compare the values of the other parameters in the status panel with values that you recorded previously.
4. Set up for ESI, APCI, APPI, or NSI operation as described in **Finnigan LTQ Getting Started**.

> **Note.** You do not need to calibrate or tune the LTQ each time you restart the LTQ.
>
> ***Calibration parameters*** are instrument parameters whose values do not vary with the type of experiment. You need to calibrate the LTQ perhaps once a month, and check the calibration once a week. Refer to **Finnigan LTQ Getting Started** for a procedure for calibrating the LTQ.
>
> ***Tune parameters*** are instrument parameters whose values vary with the type of experiment. You need to tune the LTQ (or change the Tune Method) whenever you change the type of experiment. Refer to **Finnigan LTQ Getting Started** for procedures for tuning the LTQ in the ESI or APCI mode. (Note that LTQ comes with several standard Tune Methods specific for various experimental conditions, so that tuning is often not required for many types of experiments.)

5.5 Resetting the MS Detector

If communication between the MS detector and data system computer is lost, it may be necessary to reset the MS detector using the Reset button on the power panel. When you press the Reset button (for 3 s), an interrupt in the embedded computer is created. This causes the embedded computer to restart in a known (default) state. See Figure 5-1 on page 5-2 for the location of the Reset button.

The procedure given here assumes that the MS detector and data system computer are both powered on and operational. If the MS detector, data system computer, or both are off, refer to the topic **Starting Up the System after a Complete Shutdown** on page 5-6.

To reset the MS detector, press the Reset button located on the power panel for 3 s. Make sure the Communication LED is extinguished before releasing the Reset button. When you press the Reset button (for 3 s), the following occurs:

- An interrupt on the embedded computer causes the CPU to reboot. All LEDs on the front panel of the MS detector are off except the Power LED.
- After several seconds, the Communication LED is illuminated yellow to indicate that the data system and the MS detector are starting to establish a communication link.
- After several more seconds, the Communication LED is illuminated green to indicate that the data system and the MS detector have established a communication link. Software for the operation of the MS detector is then transferred from the data system to the MS detector.
- 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.

5.6 Resetting the Tune and Calibration Parameters to their Default Values

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

> **Note.** Make sure that the problems that you are 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.

1. 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.
2. To optimize the LTQ system parameters (that is, to calibrate or tune the system), perform the calibration or tune procedure as described in **LTQ Getting Started**.

5.7 Resetting the Data System

There are two ways to reset the data system:

- By using the Windows XP shutdown and restart procedure
- By pressing the reset button on the personal computer

Resetting the Data System by Using the Windows XP Shutdown and Restart Procedure

If possible, use the Windows XP shutdown and restart procedure to shut down and restart the data system so that Windows XP can properly close applications and save changes to files.

To reset the data system by using the Windows XP shutdown and restart procedure, proceed as follows:

1. Choose **Start > Shut Down** from the Windows XP task bar. The Shut Down Windows dialog box appears.
2. Select the Restart The Computer option button, and then click on **Yes** to start the Windows XP shutdown and restart procedure.
3. Observe the Windows XP shutdown and restart procedure on the monitor.
4. Press **<Ctrl>-<Alt>-<Del>** when you are prompted to do so. Then, click on **OK** or enter your password (if you have one) in the Logon Information dialog box to complete the shutdown and restart procedure.

> **Note.** The communications link between the data system and the MS detector should be automatically reestablished after you reset the data system. When this occurs the Communication LED on the front panel of the MS detector is illuminated yellow and then green. If the system is unable to reestablish the communications link, press the Reset button (for 3 s) on the power panel of the MS detector.

Resetting the Data System by Using the Reset Button on the Personal Computer

If you are unable to reset the data system by using the Windows XP shutdown and restart procedure, proceed as follows:

1. Press the reset button on the personal computer.
2. Observe the Windows XP shutdown and restart procedure on the monitor.

3. Press **<Ctrl>-<Alt>-<Del>** when you are prompted to do so. Then, click on **OK** or enter your password (if you have one) in the Logon Information dialog box to complete the shutdown and restart procedure.
4. When the shutdown and restart procedure has completed, choose **Start > Programs > Xcalibur > LTQ Tune** to display the Tune Plus window.

Note. The communications link between the data system and the MS detector should be automatically reestablished after you reset the data system. When this occurs the Communication LED on the front panel of the MS detector is illuminated yellow and then green. If the system is unable to reestablish the communications link, press the Reset button (for 3 s) on the power panel of the MS detector.

5.8 Turning Off Selected MS Detector Components

There are five ways that you can turn off some or all of the MS detector components

- Turn off individual MS detector components from the Tune Plus window. Turning off individual MS detector components might be necessary when you are troubleshooting or when you are running certain diagnostic procedures.
- Place the MS detector in Standby. Standby is the normal condition to leave the MS detector in when it is not in use. Choose **Control > Standby** (or toggle the On/Standby button) from the Tune Plus window to place the MS detector in Standby.
- Place the MS detector in the Off condition. The Off condition is similar to Standby, except all high voltage components of the MS detector are turned off. Choose **Control > Off** from the Tune Plus window to place the MS detector in the Off condition.
- Place the electronics service switch in the Service position. The electronics service switch allows you to perform maintenance procedures involving non-vacuum system components of the MS detector.
- Place the main power circuit breaker switch in the Off (O) position. Placing the main power circuit breaker switch in the Off (O) position removes all power to the MS detector, including the vacuum system.

The on/off status of MS detector components, voltages, and gas flows is summarized in Table 5-1.

Table 5-1. On/Off Status of MS Detector Components, Voltages, and Gas Flows

MS detector component	Standby 	Off 	Electronics service switch in Service position	Main power circuit breaker switch in Off (O) position
Electron multiplier	Off	Off	Off	Off
Conversion dynode	Off	Off	Off	Off
Mass analyzer RF/waveform voltages	Off	Off	Off	Off
Mass analyzer dc offset voltage	**On**	Off	Off	Off
Ion optics multipoles RF voltages	Off	Off	Off	Off
Ion optics multipoles dc offset voltages	**On**	Off	Off	Off
Ion optics lens	**On**	Off	Off	Off
Tube lens	**On**	Off	Off	Off
Ion transfer capillary heater	**On**	On	Off	Off
Ion transfer capillary dc offset	**On**	Off	Off	Off
Corona discharge needle	Off	Off	Off	Off
APCI vaporizer	Off	Off	Off	Off
ESI needle	Off	Off	Off	Off
Sheath gas	Off	Off	Off	Off
Auxiliary gas	Off	Off	Off	Off
Sweep gas	Off	Off	Off	Off
Helium damping gas	**On**	**On**	**On**	**On**
Vent valve	Closed	Closed	Closed	**Open** (after 30 s)
Turbomolecular pump	**On**	**On**	**On**	Off
Rotary-vane pump	**On**	**On**	**On**	Off
Turbomolecular Pump Controller	**On**	**On**	**On**	Off
Power supply, electron multipliers/conversion dynodes	Off	Off	Off	Off
Power supply, 8 kV	Off	Off	Off	Off
Power supply PS1	**On**	Off	Off	Off
Power supply PS2	**On**	Off	**On**	Off

Table 5-1. On/Off Status of MS Detector Components, Voltages, and Gas Flows , continued

MS detector component	Standby 	Off 	Electronics service switch in Service position	Main power circuit breaker switch in Off (O) position
Power supply, +300 V dc	**On**	Off	Off	Off
Fan, turbomolecular pump	**On**	**On**	**On**	Off
Fan, RF coil	**On**	**On**	Off	Off
Fans, electronics tower	**On**	**On**	**On**	Off
Convectron gauge	**On**	**On**	Off	Off
Ion gauge	**On**	**On**	Off	Off

Chapter 6
Diagnostics and PCB and Assembly Replacement

Many of the MS detector components can be tested by the LTQ diagnostics. Thermo Electron's service philosophy for the LTQ system calls for troubleshooting to the lowest part, assembly, PCB, or module listed in the **Replaceable Parts** chapter. You should replace LTQ components when indicated by the LTQ diagnostics, by Thermo Electron Technical Support, or by a Thermo Electron Customer Support Engineer.

This chapter covers the following topics:

- Running the LTQ diagnostics
- Replacing a fuse in the MS detector
- Replacing a power supply in the MS detector
- Replacing a PCB or assembly in the MS detector

6.1 Running the LTQ Diagnostics

The LTQ diagnostics is used to test the major electronic circuits within the instrument and indicate whether the circuits pass or fail the tests. If there is a problem with the instrument electronics, the LTQ diagnostics can often locate the problem. You can then often correct the problem yourself by replacing a faulty PCB or assembly.

The LTQ diagnostics does not diagnose problems that are not electrical in nature. For example, it does not diagnose poor sensitivity due to misaligned or dirty components or to improper tuning. Therefore, it is important to have someone who is familiar with system operation and basic hardware theory run the diagnostics and use it to assist in isolating any problems.

Before running the diagnostics, you should consider the following:

- Did the system fail when you were running samples?
- Did problems occur after you performed maintenance on the instrument, data system, or peripherals?
- Did you change the system's configuration, cables, or peripherals just before the problem occurred?

If the answer is yes to the first item above, there is the possibility of a hardware failure, and running the diagnostics is appropriate.

If the answer is yes to one of the last two items above, the problem is probably mechanical, not electrical. Reverify that alignment, configurations, and cable connections are correct before you run the LTQ diagnostics.

To run the LTQ diagnostics, proceed as follows:

1. Tune the ring electrode and octapole RF voltages as described in the topic **Tuning the Ring Electrode and Octapole RF Voltages** in the **MS Detector Maintenance** chapter.
2. In the Tune Plus window, choose **Diagnostics > Diagnostics**. (To open Tune Plus, choose **Start > Programs > Xcalibur > LTQ Tune**.) The Diagnostics dialog box appears. See Figure 7-1.
3. Select one of the following options:
   - To test all of the electronic subsystems (that is, the vacuum system, power supplies, lenses, ion detection system, and RF voltage electronics), click on the **All** tab and select the **Everything** option.
   - To test an individual subsystem, click on the tab corresponding to that subsystem and select the appropriate options.
4. Select how many times you want to run the tests, and whether or not you want to print reports or to stop on a failure.
5. Click on the **Start** button to start the diagnostics.

LTQ starts testing and displays a chronological log of all diagnostic tests in the Testing text box. Once testing for a specific subsystem is completed, LTQ displays either Pass or Fail in the Results group box. If the LTQ diagnostics indicates a problem, perform the maintenance procedure indicated by the LTQ diagnostics, by Thermo Electron Technical Support, or by a Thermo Electron Customer Support Engineer. For more information on the LTQ diagnostics, refer to the LTQ online Help.

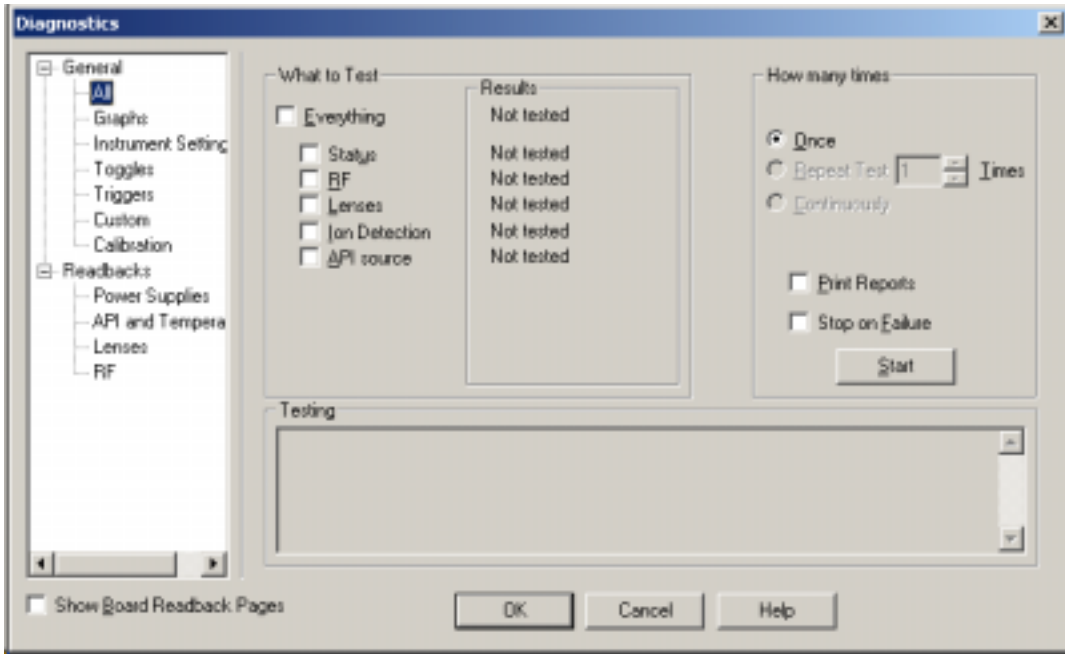


Figure 6-1. Diagnostics dialog box

6.2 Replacing a Fuse

Fuses protect the various circuits by opening the circuits whenever overcurrent occurs. On the MS detector the fuses are located on the Interlock PCB and Source PCB. The function and current rating of the various fuses are listed in Table 6-1.

Check fuses when power is lost to a fused subsystem.

CAUTION. Always shut down the system and disconnect the power cord before you replace fuses.

Table 6-1. MS detector fuses

Location	Fuse	Circuit	Description	P/N
Interlock PCB	F1,F3	APCI vaporizer heater	3.15 A, Type F, 5 x 20 mm, 250 V	00006-10510
Interlock PCB	F2, F4	220 Vac	6.3 A, 250 V	00006-11450
Source PCB	F3		4.0 A, 250 V	00006-11420

Caution. Use only the fuses specified in Table 6-1. Never replace a fuse with a fuse of a different type, voltage, or current rating.

6.3 Replacing Power Supplies

The following power supplies are easily accessed from the front of the LTQ. See Figure 6-3.

- PS1 power supply
- PS2 power supply
- 300 V power supply
- 8 kV power supply

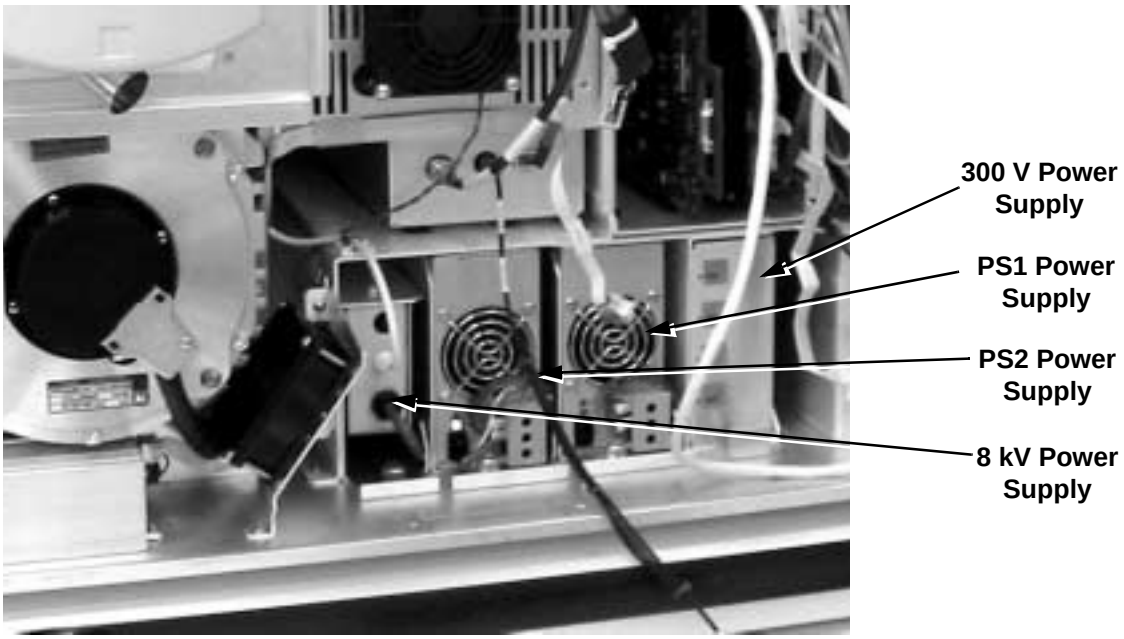


Figure 6-2. Power supplies

To replace the PS1 power supply (P/N 97055-60014S), PS2 power supply (P/N 97055-60015S), 300 V power supply (P/N 97055-98001), or the 8 kV power supply (P/N 97055-60033), proceed as follows:

1. Shut down and vent the system as described in the topic **Shutting Down the System Completely** in the **System Shutdown, Startup, and Reset** chapter.

CAUTION. Make sure that the LTQ power cord is unplugged before you proceed.

2. Open the right front door of the MS detector by loosening the Allen screw on the right door with an Allen wrench.

3. If necessary, remove the left front cover as follows:
   a. If necessary, remove the Ion Max ion source as described in the topic **Removing the Ion Max Ion Source** on page 4-12.
   b. Unscrew the two fasteners that secure the left front cover to the vertical beam.
   c. Move the left front cover up by 0.2 in., and then pull it out enough to access the cables that connect to the back.
   d. Disconnect the cables and remove the cover.
4. If necessary, remove the vertical beam.
5. The power supplies in the tower have bulkhead connectors on the back. To remove a power supply, loosen the fastener that holds it to the chassis and then carefully tug on the power supply to remove it as a module.
6. Unpack the new power supply. Retain the packing materials so that you can pack and ship the defective switching power supply assembly to the Thermo Electron Repair Center in San Jose. **Be sure to note the apparent problem or symptoms on the enclosed forms.**
7. Slide the new power supply into the space occupied by the old power supply. Push carefully on the power supply to seat the connectors in the rear.
8. Tighten with a Phillips screwdriver the fastener that holds the power supply to the tower.
9. If necessary, reinstall the vertical beam if you removed it in step 4.
10. If necessary, reinstall the left front cover if you removed it in step 3, as follows:
    a. While holding the left front cover next to the left side of the MS detector, reconnect the cables to the back of the cover.
    b. Reinstall the left front cover on the MS detector and tighten the two fasteners that secure the left front cover to the vertical beam.
    c. If necessary, reinstall the Ion Max ion source as described in the topic **Reinstalling the Ion Max Ion Source** on page 4-19.
11. Close the right front door of the MS detector. Tighten the Allen screw on the on the right front door with an Allen wrench.
12. Restart the system as described in the topic **Starting Up the System After a Complete Shutdown** in the **System Shutdown, Startup, and Reset** chapter.
13. Run the LTQ diagnostics to verify that the system is operational.

6.4 Replacing PCBs in the MS Detector

The LTQ electronic assemblies are close-packed to minimize the size of the system. Due to the complexity of removing and reinstalling many of the LTQ PCBs, we recommend that a Thermo Electron Field Service Engineer replace the electronic assemblies.

PCBs and assemblies in the MS detector are shown in Figure 6-3

CAUTION. Shutdown the system and unplug the power cord before you access PCBs and electronic assemblies.

Caution. To prevent damage to the electronics due to electrostatic discharge, attach an electrostatic discharge (ESD) strap to your wrist before handling PCBs.

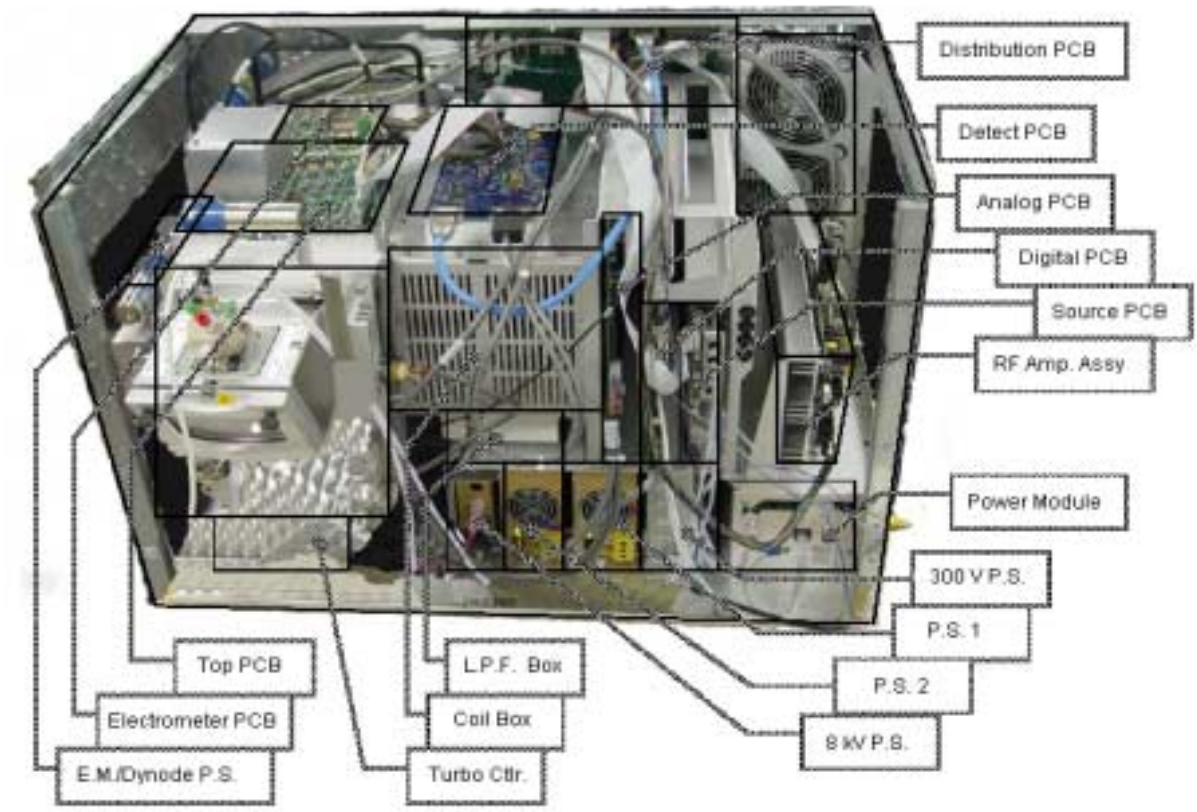


Figure 6-3. LTQ PCBs, power supplies, and electronic modules

Chapter 7
Replaceable Parts

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

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

> **Note**. Some parts are also available as exchange parts. An exchange part is a refurbished part that can be purchased at a discounted price. Exchange parts are specified by placing *EX* in front of the part number. For example, EX70111-60002S.

This chapter contains part numbers for the following:

- MS Detector
- Data system hardware
- Manuals
- Accessory kit
- Metal needle kits
- Fittings, ferrules, and sample loops

7.1 MS Detector

Replaceable parts are available to support the following:

- ESI source
- APCI source
- Ion source interface
- Ion guides
- Mass analyzer
- Divert/inject valve
- Syringe pump
- Turbomolecular pump
- Forepump
- Pressure gauges
- Vacuum system assemblies
- Vacuum manifold O-rings
- Vent valve
- Power supplies
- Printed circuit boards (PCBs)
- RF control / detection assemblies
- Cables
- Fans

ESI Source

Please note that not all parts are available for purchase separately, some parts may only be available for purchase as part of a kit or assembly.

ESI Probe OPTON-20011
- Body-probe manifold 97055-20215
- Nozzle-ESI probe 3-port 97055-20146
- Fitting, union, ZDV, 1/4-28, PEEK, black 00109-00304
- Needle, metal, 32 gauge, ESI 97055-20217
- Contact, Battery, BECU, 0.598 mml, 0.02 ohm@4A 00004-21402
- Seal STD needle 5000 series 00950-00952
- Needle, D PNT 26 gauge, 2""L, .24D washer 00950-00990
- O-ring 00.438ID 1/16 in. Viton 00107-05575
- Connector receptacle, high voltage, shielded 00004-89626
- Ferrule .012ID KEL-F HPLC 00101-18116
- Fitting, Fingertight 2 Upchurch 00101-18195
- Fitting, plug 1/4-28 TEFZEL HPLC 00101-18075
- O-ring 0.676 ID 1/16 TH VI 00107-05710
- O-ring 00.125ID 1/16TH VI 00107-02550
- Assembly-resistor contact-ESI probe 97055-60058
- Sleeve-resistor 97055-20147
- Resistor FXD CC 1/4W 22M 5% 00015-27820
- Fitting HPLC adptr 10-32 × 1/4-28KEL 00101-18080
- Tubing fused-silica .10 ID × .19 00106-10499
- Ferrule .008 ID KEL-F HPLC 00101-18114

Safety Sleeve Kit 70005-62015
- Ferrule .27 ID PEEK HPLC 00101-18119
- Tube .009IDx. 024 OD × 10" natural PEEK 00301-22806
- Instructions safety sleeve 70005-97009
- FTG Fingertight 2 Upchurch 00101-18195
- FTG, nut, finger, HPLC, 10-32, PEEK 00101-18081

Stainless steel needle kit, 32 gauge OPTON-20014

Stainless steel needle kit, 34 gauge OPTON-20015

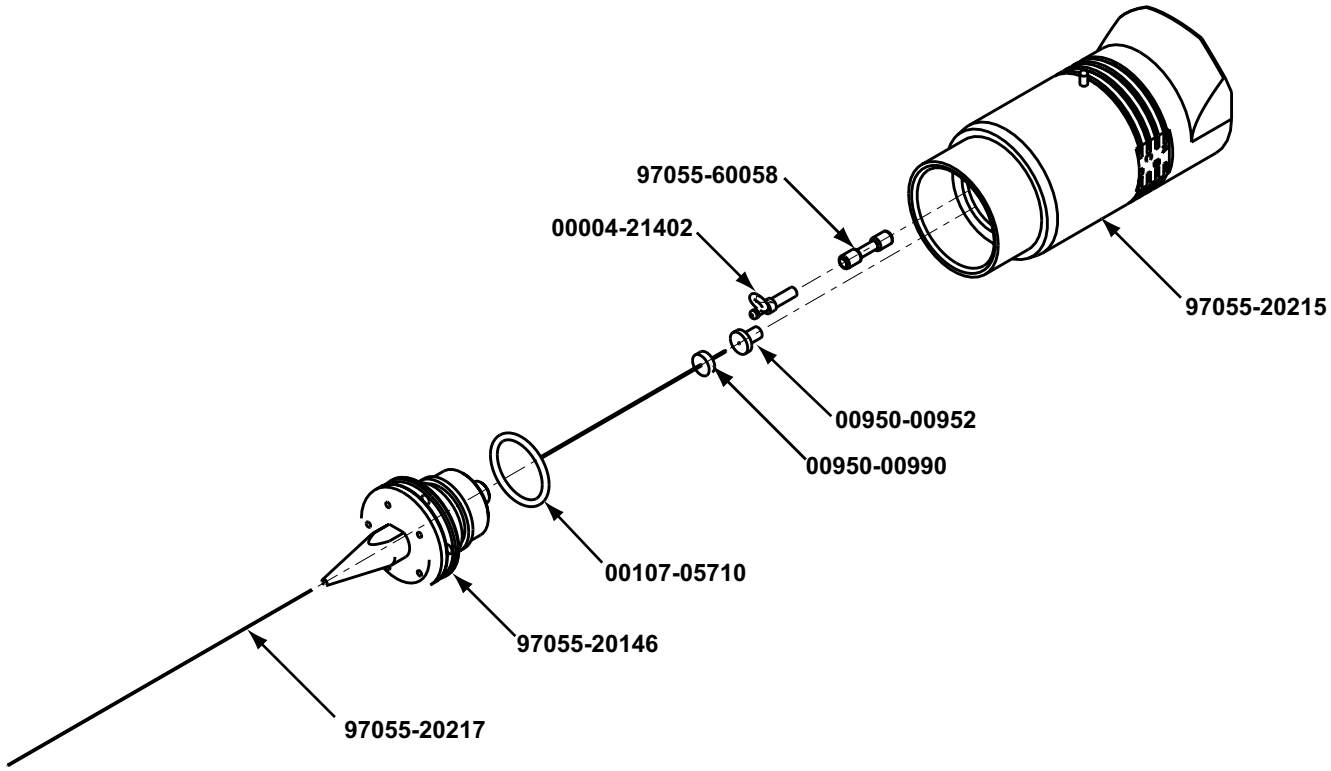


Figure 7-1. Exploded view of the ESI probe

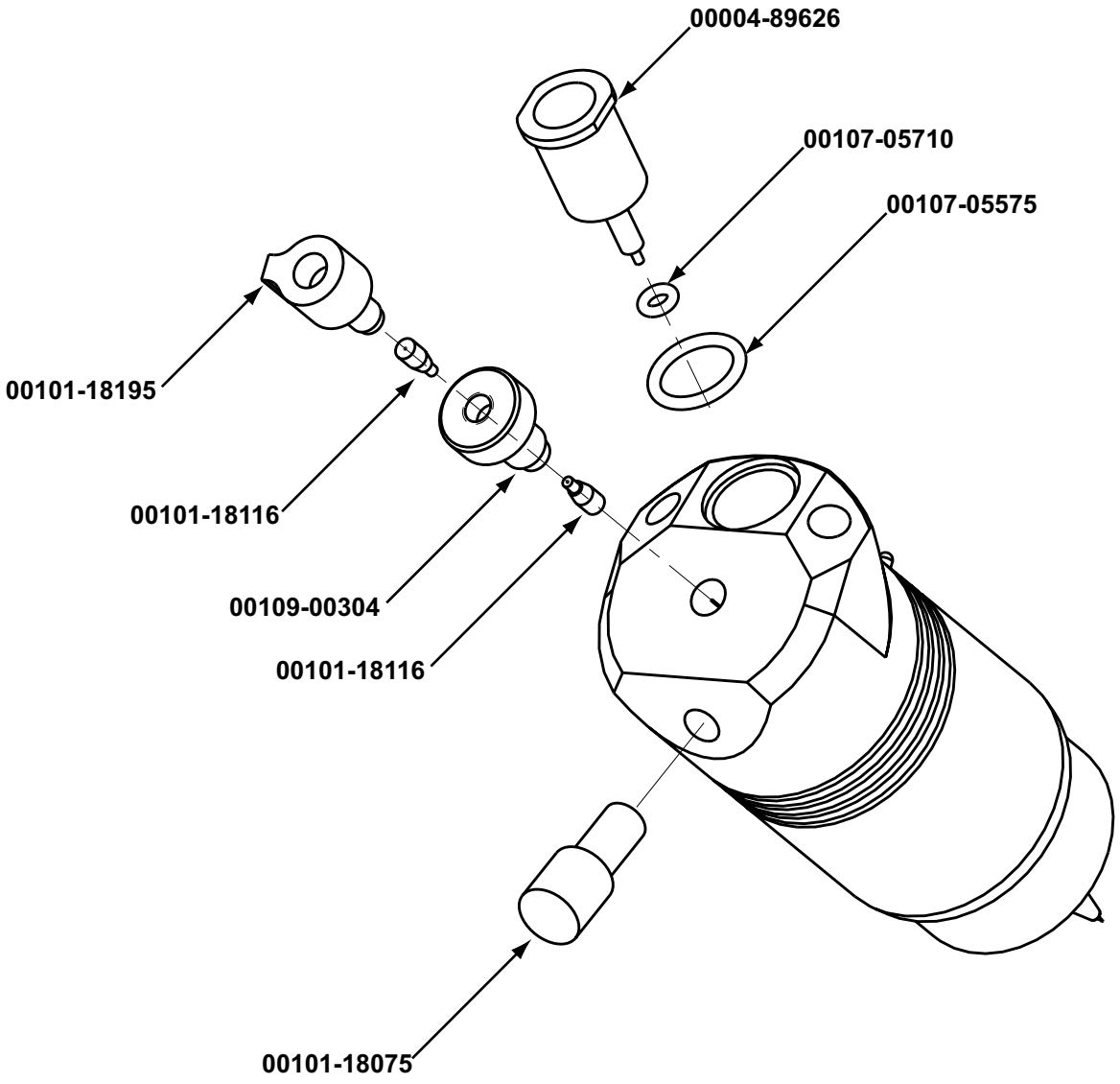


Figure 7-2. Replaceable parts for the ESI probe

APCI Source

APCI probe OPTON-20012

APCI probe nozzle assembly 97055-60089
- Ferrule, .016ID PEEK HPLC 00101-18120
- Tubing, fused silica 150U X 390U 00106-10498
- O-ring, .239 1/16th Viton 00107-04000
- O-ring, 00.312 ID=5/16 1/16 00107-04500
- O-ring, 00.500 ID 1/16TH VI 00107-05600
- Fitting, 10-32 male nut PEEK 70005-20220
- Fitting, APCI flange 70005-20250
- Nozzle, APCI probe 97055-20221

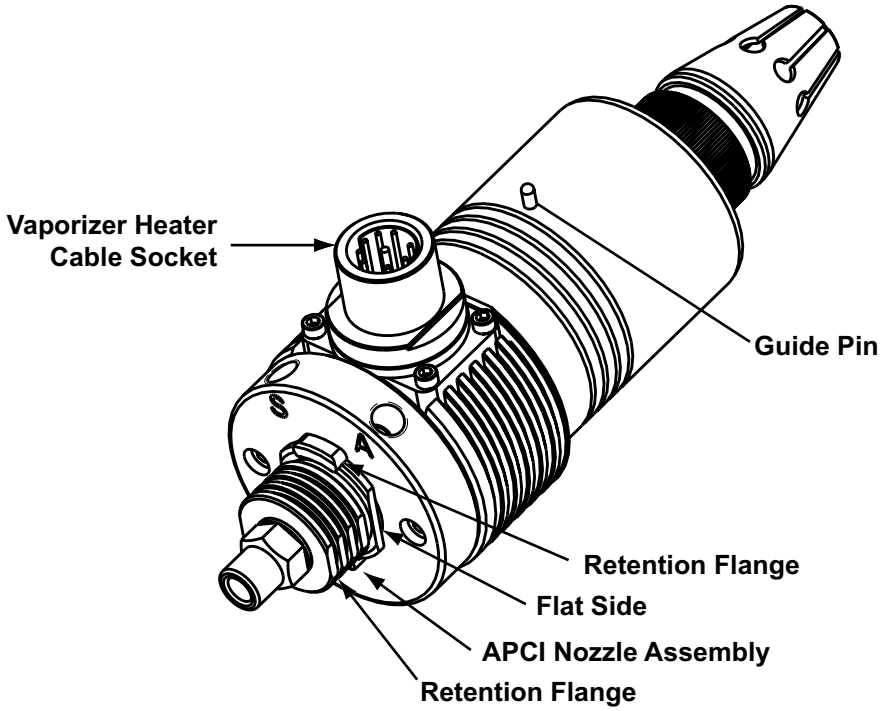


Figure 7-3. APCI Probe Assembly (OPTON-20012)

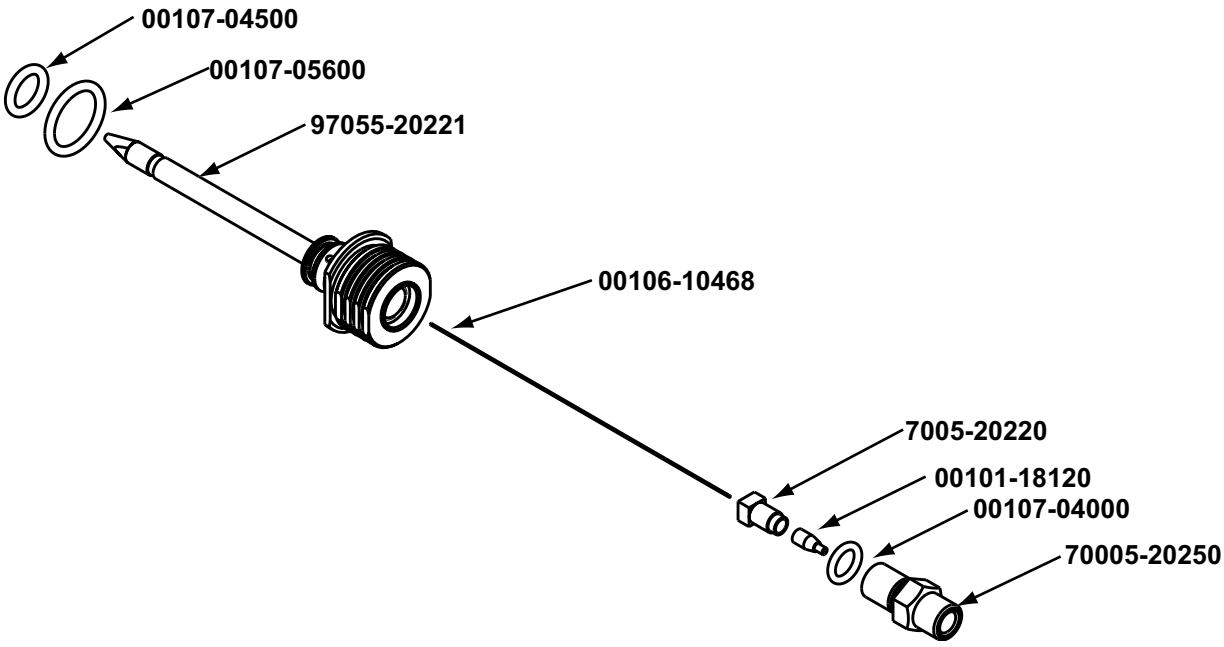


Figure 7-4. APCI probe nozzle assembly (P/N 97055-60089)

Ion Source Interface

Ion Source Interface Assembly 97055-60040
Contact socket for 0.048 x 0.064D pin..... 00004-89652
O-ring,2-033 Viton V884 (2 x 1/16) 00107-01-00006
O-ring, 2.625ID x3/32, AS-146, Viton.....00107-11002
O-ring, 2-74 x 0.063, 2-039 Viton..... 00107-12550
O-ring, 0.30ID x 0.054, Kalrez, CMPD, 4079 00107-12750
Plunger ball, 6-40 x 0.31, 1lb 00201-11719
Screw, socket, 2-56 x 3/16, ss 00419-25603
Screw, 4-40 x 3/8, SHCS, vented, stainless steel 00419-44014
Screw, socket, 6-32 x 1, ss..... 00419-63216
Screw, set, socket, 6-32 x 7/8, alloy, A574 00451-63278
Screw, 2-56 x 3/32, socket head, stainless steel 00452-25612
Seal, graphite source heater.....70111-20216
Thumbnut, knurled 6-32..... 97055-20033
Seal, API cone 97055-20034
Cone, API source (sweep cone) 97055-20035
Ring, contact, support..... 97055-20036
Ring, contact backplate 97055-20052
Capillary heater assembly 97055-20074
Bush, nose cone insulator..... 97055-60043
Cage, capillary heater mount..... 97055-20065
Ion transfer capillary, 550 micron 97055-20198
Clamp socket 97055-20203
Ion sweep cone 97055-20214
Tube lens 97055-20251
Skimmer 97055-20253

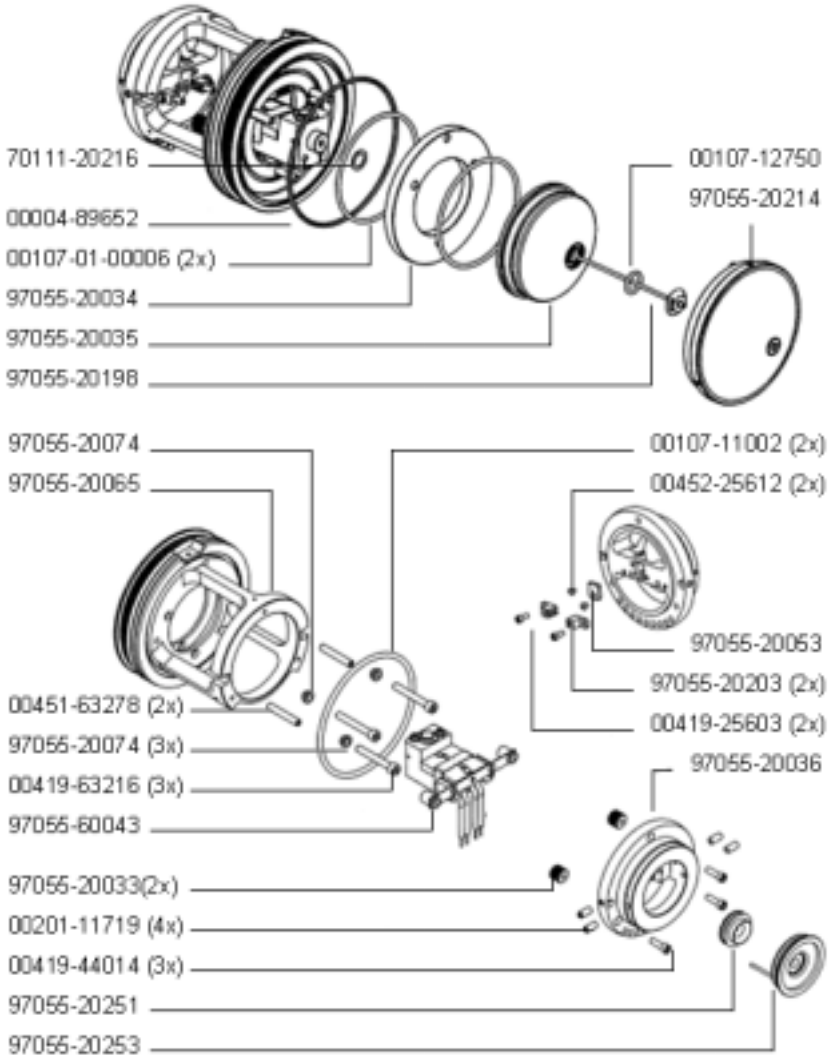


Figure 7-5. Ion source interface part numbers

Q00 Ion Guide

Q00 Ion Guide Assembly 97055-60036
O-ring, 0.101ID x 0.070, Viton 00107-02456
O-ring, 2-148, Viton 884 00107-15542
Plunger ball, ¼-20 x 0.53, 4lb 00201-11716
Plunger ball, 6-40 x 0.31, 1lb 00201-11719
Screw, socket HD, CAP, 4-40 x 3/8, ss 00419-44010
Screw, socket, 6-32 x ¼, ss 00419-63204
Lens, L1 mount 97055-20026
Rod, threaded guide 97055-20050
Cage, outer contact support 97055-20053
Manifold, API gas inlet 97055-20067
Quadrupole, Q00, large R0 97055-20106
Latch block, probe housing 97055-20128
Cage Contact Ring Assembly 97055-63082
Link Set Q0-L0 Assembly 97055-63080

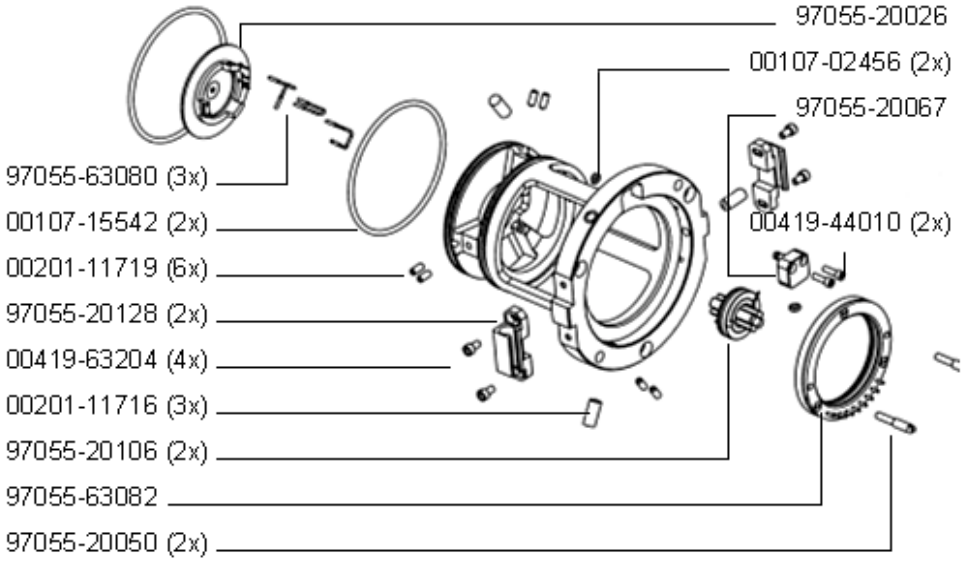


Figure 7-6. Q00 ion guide part numbers

Q0 and Q1 Ion Guides

Thumb screws, 10-32	97000-20235
Lens L1	97055-20022
Gate lens	97055-20023
Multipole bracket	97055-20054
Q1 octapole	97055-60034
Q0 quadrupole	97055-60035

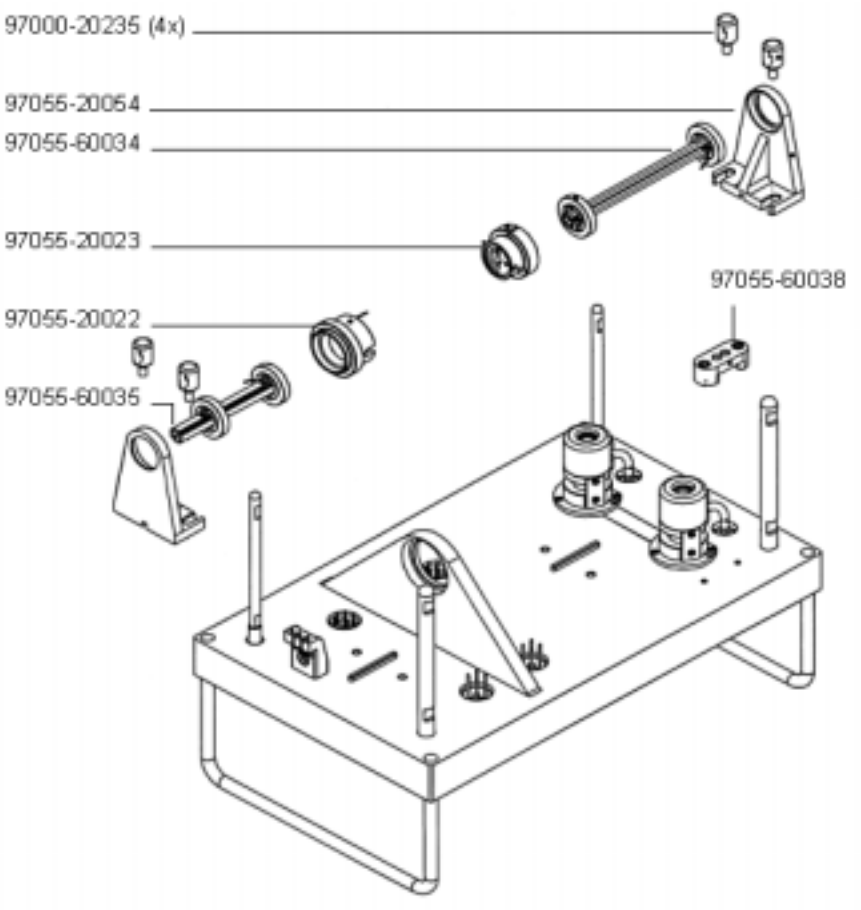


Figure 7-7. Q0 and Q1 ion guides part numbers

Mass Analyzer

Mass analyzer assembly, linear ion trap 97055-60039

Electron Multiplier

Electron multiplier assembly 96000-60036

Coil Module

RF coil and PCB Assembly 97055-60091

Divert/Inject Valve

Divert/inject valve (Rheodyne MM501, 2 position, 6 port) 00110-03-00001

Syringe Pump

Syringe pump.....97055-98006

Turbomolecular Pump

Turbomolecular pump insert (Leybold TW 400/300/25) EX00108-10022

Turbomolecular pump controller (Leybold TDS)..... 00108-10012

Forepump

Forepump Kit.....70111-62014
- Forepump (mechanical pump), E2M30, 650 L^3/min, 220V AC..... 00108-02655
- Vacuum hardware clamp, KF-20/25..... 00102-10020
- Pump hardware centering ring 00108-02011
- Mist Filter..... 00108-02-00002
- Hose clamp, band 00201-03810
- PVC vacuum hose reinforced, 1.5-in ID 00301-24163
- Tool, extraction, minifit..... 00725-00050
- Drain oil return kit..... 00960-01-00007
- Adapter, pump roughing line.....70111-20210

Pressure Gauges

Convectron gauge 00105-00501

Ion gauge..... 97055-62001

Vacuum Accessories

Hose and Accessories Kit 97055-62007
PVC vacuum hose reinforced, 1.5-in. ID 00301-24163
Manifold, 3-port, 1.5-in. 97055-20222
Flange, NW40, long 00108-02-00003
Clamp, NW32/40, swing 00108-02-00004
Ring, centering 00108-02-00005
Adaptor, pump roughing line 70111-20210
Hose clamp, band 00201-03810
Pump hardware centering ring 00108-02011
Vacuum hardware clamp KF-20/25 00102-10020

Vacuum Manifold O-Rings

O-ring, 0.31-in. ID × 1/16 00107-05000

O-ring, 4.5-in. ID × 1/8, Viton 00107-14500

O-ring, 6.48-in. ID × 1/8, Viton 00107-15270

O-ring, 7.734-in. ID × 1/8, Viton 00107-15544

O-ring, 5.86-in. ID × 1/8, Viton 00107-15550

O-ring, split chamber 97055-40005

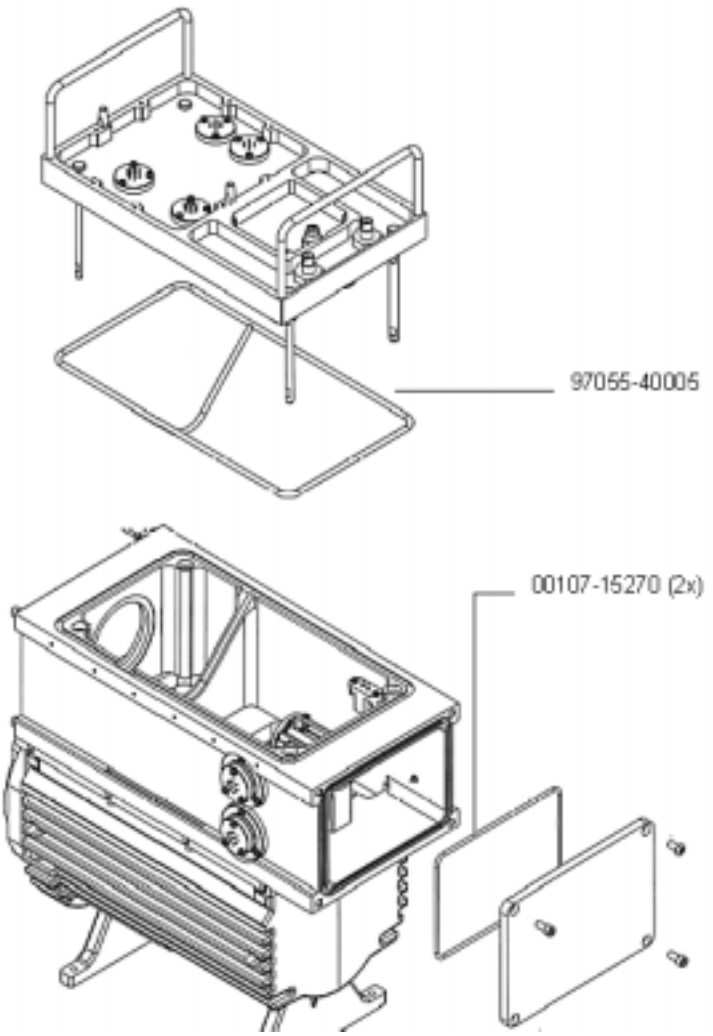


Figure 7-8. Vacuum manifold O-rings part numbers

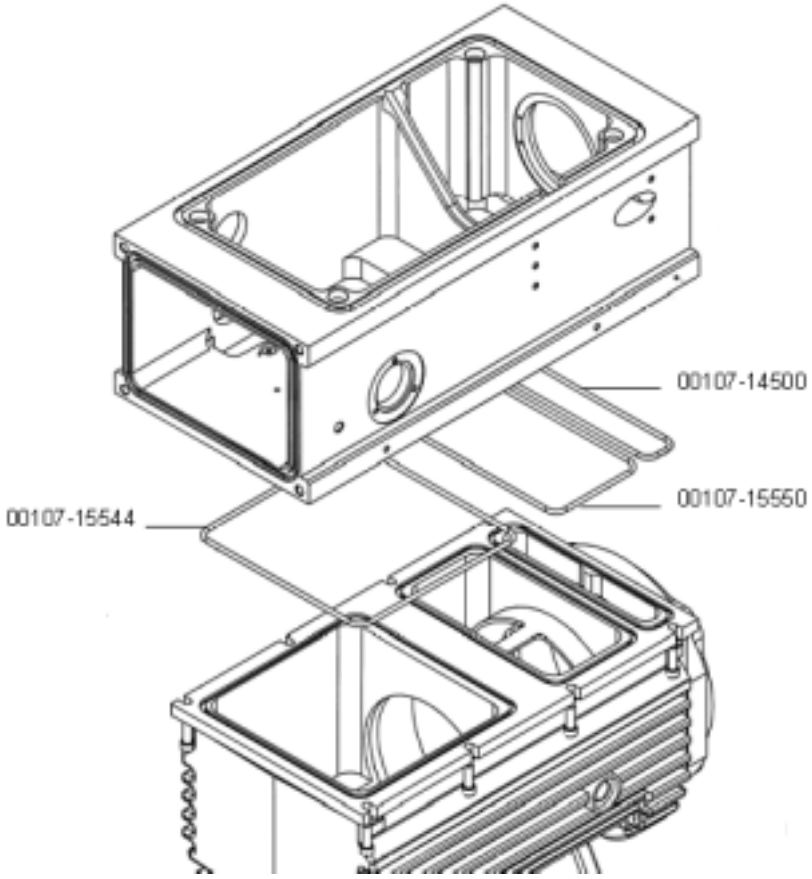


Figure 7-9. Vacuum manifold O-rings part numbers

Vent Valve

Vent valve assembly 97055-60084

Power Supplies

PS1, +60 V (6 A), +5 V (35 A), ±15 V (14 A) 97055-60014S
PS2, +36 V (10 A), ±24 V (8.5 A), +28 V (6.7 A) 97055-60015S
8 kV Power Supply 97055-60033
15 kV dual Electron Multiplier/Conversion Dynode power supply 97055-98002
300 V power supply 97055-98001
Power module (available as exchange) 97055-60006S

Printed Circuit Boards (PCBs)

Source PCB (available as exchange) 70111-61053S
Interlock PCB 70111-61060S
Digital PCB (available as exchange) 97055-61010S
Distribution PCB 97055-61020S
Analog PCB (available as exchange) 97055-61030S
Top Cover PCB (available as exchange ..... 97055-61040S)
I/O PCB 97055-61070S
Front Panel PCB 97055-61110S
Electrometer PCB 97055-61190S
RF Detector PCB (available as exchange) 97055-61200S
Divert/Inject Valve PCB 97055-61140S
RF Amplifier PCB 97055-61180S

Cables

Ethernet (Power Module) to Digital PCB 00012-70064
Power Module wire set 97055-63000
Interlock PCB to Power Module bulkhead 97055-63004
Interlock PCB 220 Vac In 97055-63006
I/O PCB to Power Module Elcon adapter 97055-63008

Cable, Power/Signal Distribution to Power Module and Digital PCB 97055-63106

Fans

Fan, 100 CFM, 24V dc, located on fan housing assembly 00013-00243

Fan, 21 CFM, 24V dc, located on coil module assembly and adjacent to the turbomolecular pump 97055-63083 .....

Fan filter..... 97055-20254

7.2 Manuals

Finnigan LTQ Preinstallation Requirements Guide.....97055-97010

Finnigan LTQ Getting Connected.....97055-97011

Finnigan LTQ Getting Started.....97055-97012

Finnigan LTQ Hardware Manual.....97055-97013

7.3 Accessory Kit

Accessory Kit.....97055-62003
- Connector, receptical, 6 p.....00004-06-00008
- Connector, receptical, 8 p.....00004-21507
- Connector, acc., cable housing, 8 p.....00004-21509
- Fuse, 3.15 A, 250 V (Interlock PCB fuses F1 and F3), (4 each) 00006-10510
- Fuse, 4 A, 250 V (Source PCB fuse F3), (4 each) 00006-11420
- Fuse, 6.3 A, 250 V (Interlock PCB fuses F2 and F4), (4 each) 00006-11450
- Cable, serial.....00012-51086
- Fitting, Swagelok, Adapt-M, 1/8 x 1/4-in. 00101-01740
- Fitting, ferrule, HPLC, reducer, 1/8 x 16-in. 00101-02-00002
- Fitting, Swagelok, bulkhead, 1/8 in. 00101-02102
- Fitting, ferrule, Swagelok, Back, 1/8 in. (2 each) 00101-02500
- Fitting, ferrule, Swagelok, Back, 1/4 in. (2 each) 00101-04000
- Fitting, tube, bulkhead, 1/8 in. 00101-04-00001
- Fitting, comp., elbow, 1/8 in. 00101-04-00002
- Fitting, ferrule, Swagelok, Front, 1/8 in. (2 each).....00101-08500
- Fitting, ferrule, Swagelok, Front, 1/4 in. (2 each).....00101-10000
- Fitting, Swagelok, Nut, 1/4 in., brass.....00101-12500
- Fitting, Swagelok, O-seal, 1/4 in.....00101-13510
- Fitting, Swagelok, Nut, 1/8 in., brass (2 each).....00101-15500
- Fitting, nut, HPLC, flangeless (2 each).....00101-18084
- Ferrule, 0.008 in. ID, KEL-F, HPLC (4 each).....00101-18114
- Ferrule, 0.016 in. ID, PEEK, HPLC (4 each).....00101-18120

Fitting, Fingertight 2, Upchurch 00101-18195
Ferrule, Fingertight 2, Upchurch (3 each) 00101-18196
Fitting, flangeless, 1/8 in. Upchurch..... 00101-18198
Fitting, ferrule, 1/8 in. Tefzel..... 00101-18199
Fitting, flangeless, 1/8 in. Blue Delrin..... 00101-18200
Fitting, HPLC Union, 0.010 orifice, PEEK 00101-18202
Fitting, HPLC, Tee, 0.020 orifice, PEEK 00101-18204
Fitting, ferrule, 1/8 in. Tefzel, short..... 00101-18223
Tubing, Teflon, 0.125 mm OD × 0.03 w (2 each) 00101-50000
Tubing, PFA, 0.25 mm OD × 0.062 w (2 each)..... 00101-50100
Fitting, Tee, barbed, 1.0-in..... 00102-10120
Nut, flangeless, electrospray, 1/16-in. 00102-10146
Ferrule, Tefzel, electrospray, 1/16-in. 00102-10148
Fitting, union, tube,bulkhead, 1/4-in. 00103-01-00001
Fitting, tube, straight, 1/8-in. x 10-32..... 00103-10990
Tubing, fused silica, 0.150 mm × 0.390 mm 00106-10498
Tubing, fused silica, 0.10 mm ID × 0.19 mm OD 00106-10499
Tubing, fused silica, 0.05 mm ID × 0.19 mm OD, deactivated..... 00106-10502
Tubing, fused silica, 0.11 mm ID × 0.4 mm OD, deactivated 00106-10504
O-ring, 2.5-in., Viton 00107-01-00002
O-ring, 0.218-in., Viton (2 each) 00107-01-00004
O-ring, 2.033-in., Viton 00107-01-00006
O-ring, 3/16-in. (6 each) 00107-01-00009
O-ring, 0.926-in., Viton 00107-01-00013
O-ring, 0.101 ID, Viton (6 each)..... 00107-02456
O-ring, 0.174 ID, Viton 00107-02464
O-ring, 0.125 ID, Viton (2 each)..... 00107-02550
O-ring, 0.239 ID, Viton (3 each)..... 00107-04000
O-ring, 0.312 ID 00107-05000
O-ring, 0.375 ID 00107-07000
O-ring, 0.468 ID, Viton..... 00107-07600
O-ring, 0.5 ID, Viton..... 00107-08000
O-ring, 0.737 ID, Viton (2 each)..... 00107-10056
O-ring, 0.739 ID, Viton 00107-10100
O-ring, 1.37 ID, Viton 00107-10400
O-ring, 0.30 ID, Kalrez 00107-12750
Fitting, HPLC, nut, flangeless, 1/4-in.-28 00109-02-00002
Sample loop, 2 µL, PEEK 00110-16012
Sample loop, 20 µL, stainless steel..... 00110-22014
Sample loop, 5 µL, stainless steel..... 00110-22026
Fitting, bushing, Rheodyne (6 each)..... 2522-0066
Ferrule, tube, 1/16-in. (6 each) 2522-3830
Air duct, flexible, 1.0-in. ID 00301-08301
Oil, vacuum pump, 1 L 00301-15101
Syringe, 10 µL, Rheodyne..... 00301-19008
Syringe, 250 µL, Gas Tight, Removable needle..... 00301-19015
Syringe, 500 µL, Gas Tight, Removable needle..... 00301-19016
Tubing, Cu, refrigeration, 1/8-in. OD 16.5 ft. long 00301-22701

Tubing, PVC, unreinforced 0.005 ID × 1/16 in. OD, 10 ft. long	00301-22895
Tubing, Teflon, 0.030 in. ID × 1/16 in. OD	00301-22915
Tubing, PEEK, 0.005 ID × 1/16 in. OD, Red, 5 ft. (1.5 m long)	00301-22912
Hose, poly, spiral, PVC, superflex, 1.5 ft.	00301-24168
Cable shield, 22 gauge, 24 ft.	00302-01800
Wrench, L, hex, 4 mm	00725-00034
Troubleshooting guide, HPLC	00920-05914
Seal, STD, Needle, 5000 Series	00950-00952
Needle, D Point, 26 gauge, 2 in. long, 0.24D washer	00950-00990
Corona needle, APCI (5 each)	70005-98033
Seal, API source heater, graphite	70111-20216
Tool, ion transfer capillary removal	70111-20258
Kit, Chemicals	97000-62042
Ion transfer capillary, insert, replaceable	97055-20198
Adapter union, probe, ground	97055-20230

7.4 Metal Needle Kits

High Flow Needle Kit OPTON-20004

(Recommended for LC flow rates between 5 and 400 µL/min)

Ferrule, 0.012 in. ID, Kel-F 00101-18114
Ferrule, 0.012 in. ID, Kel-F 00101-18116
Fitting, Fingertight 2, Upchurch 00101-18195
Union, zero dead volume, 1/4-28, Upchurch 70111-20233
Blunt-tip, 32-gauge, 50 µm ID, stainless steel needle 70111-20287

Low Flow Metal Needle Kit OPTON-20005

(Recommended for LC flow rates between 500 nL/min and 10 µL/min)

Ferrule, 0.012 in. ID, Kel-F 00101-18114
Ferrule, 0.012 in. ID, Kel-F 00101-18116
Fitting, Fingertight 2, Upchurch 00101-18195
Union, zero dead volume, 1/4-28, Upchurch 70111-20233
Blunt-tip, 34-gauge, 30 µm ID, stainless steel needle 70111-20288

7.5 Fittings, Ferrules, Sample Loops, and Tubing

Ferrule, Fingertight 2, Upchurch. (for: PEEK tubing and Teflon tube) 00101-18196

Ferrule, 0.016 in. ID, PEEK, Upchurch
(for: Fused-silica capillary infusion line) 00101-18120

Ferrule, 0.012 in. ID, Kel-F, Upchurch
(for: High flow metal needle and low flow metal needle) 00101-18114

Ferrule, 0.008 in. ID, Kel-F, Upchurch
(for: Fused-silica capillary sample line). 00101-18116

Ferrule, LC, 1/16 in., stainless steel, Rheodyne 2522-3830

Fitting, Fingertight, Upchurch. 00101-18195

Fitting, Fingertight, Upchurch. 00101-18081

Fitting, adapter, Kel-F, 10-32 × 1/4-28, Upchurch
(connects directly to ESI probe inlet) 00101-18080

Nut, LC, 1/16 in., stainless steel, Rheodyne. 2522-0066

Fitting, LC union, 0.010 in. orifice, PEEK. 00101-18202

Fitting, LC TEE union, 0.020 in. orifice, PEEK 00101-18204

Fitting, adapter union, PEEK, Upchurch. 00101-18206

5 µL sample loop, stainless steel. 00110-22010

10 µL sample loop, stainless steel. 00110-22012

20 µL sample loop, stainless steel. 00110-22014

50 µL sample loop, stainless steel 00110-22016

100 µL sample loop, stainless steel. 00110-22018

500 µL sample loop, stainless steel 00110-22020

1 mL sample loop, stainless steel..... 00110-22022

Tubing, 0.15 mm ID × 0.39 mm OD fused-silica capillary (APCI sample tube)..... 00106-10498

Tubing, 0.10 mm ID × 0.19 mm OD fused-silica capillary (ESI sample tube)..... 00106-10499

Tubing, 0.05 mm ID × 0.19 mm OD fused-silica capillary (low flow ESI < 200 µL/min)..... 00106-10502

Tubing, 0.1 mm ID × 0.363 mm OD fused-silica capillary (infusion line)..... 00106-10504

Tubing, 0.075 mm ID × 0.3193 mm OD fused-silica capillary (low flow ESI).....00106-10511

Teflon tube (syringe adapter assembly)..... 00301-22915

7.6 Chemicals Kit

Chemicals Kit 97000-62042
- Met-Arg-Phe-Ala, 20 mg 00301-07709
- Ultramark 1621 00301-12200
- Caffeine, 1 mg/mL 00301-12310
- Reserpine, 1 g..... 00301-12901

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