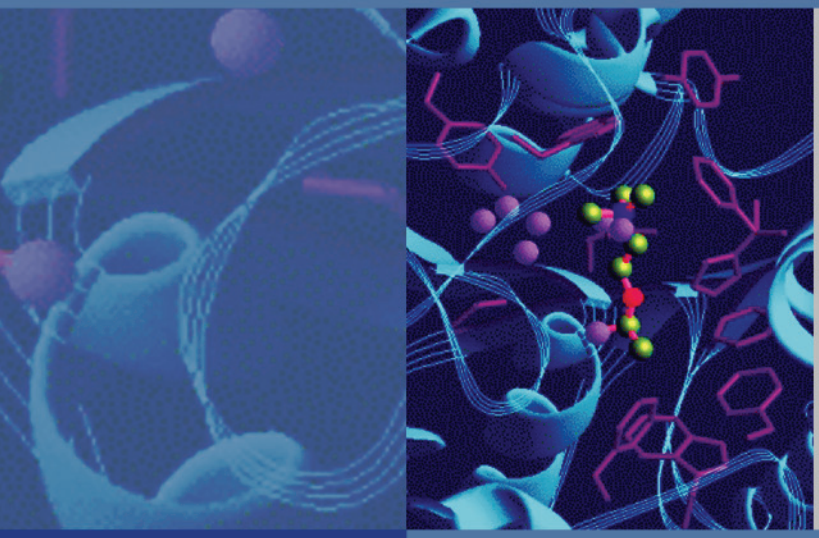

LCQ

Fleet

Hardware Manual

97055-97063 Revision A April 2007

For Research Use Only
Not for use in Diagnostic Procedures

Thermo SCIENTIFIC

Release history: Revision A, April 2007

Software revision: LCQ Fleet 2.4, Xcalibur 2.0.5 and higher, LC Devices 2.0.2

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Regulatory Compliance

Thermo Fisher Scientific performs complete testing and evaluation of its products to ensure full compliance with applicable domestic and international regulations. When the system is delivered to you, it meets all pertinent electromagnetic compatibility (EMC) and safety standards as described below.

EMC Directive 89/336/EEC as amended by 92/31/EEC and 93/68/EEC

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

EN 55011	1998, A1; 1999, A2: 2002	EN 61000-4-3	2002
EN 61000-3-2	1995, A1; 1998, A2; 1998, A14; 2000	EN 61000-4-4	1995, A1; 2000, A2; 2001
EN 61000-3-3	1995; A1; 2001	EN 61000-4-5	1995, A1; 2001
EN 61326-1	1997; A1; 1998, A2; 2001, A3; 2003	EN 61000-4-6	1996, A1; 2001
EN 61000-4-2	2001	EN 61000-4-11	1994, A1; 2001
		CISPR 11	1998, A1; 1999, A2; 2002

FCC Class A, CFR 47 Part 15 and Part 18, 2005

Low Voltage Safety Compliance

Compliance with safety issues is declared under Thermo Fisher Scientific sole responsibility.
This device complies with Low Voltage Directive 73/23/EEC and harmonized standard EN 61010-1:2001.

Changes that you make to your system may void compliance with one or more of these EMC and safety standards. Changes to your system include replacing a part or adding components, options, or peripherals not specifically authorized and qualified by Thermo Fisher Scientific. To ensure continued compliance with EMC and safety standards, replacement parts and additional components, options, and peripherals must be ordered from Thermo Fisher Scientific or one of its authorized representatives.

FCC Compliance Statement

THIS DEVICE COMPLIES WITH PART 15 OF THE FCC RULES. OPERATION IS SUBJECT TO THE FOLLOWING TWO CONDITIONS: (1) THIS DEVICE MAY NOT CAUSE HARMFUL INTERFERENCE, AND (2) THIS DEVICE MUST ACCEPT ANY INTERFERENCE RECEIVED, INCLUDING INTERFERENCE THAT MAY CAUSE UNDESIRED OPERATION.

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

Notice on Lifting and Handling of Thermo Fisher Scientific San Jose Instruments

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

Notice on the Proper Use of Thermo Fisher Scientific San Jose Instruments

In compliance with international regulations: Use of this instrument in a manner not specified by Thermo Fisher Scientific San Jose could impair any protection provided by the instrument.

Notice on the Susceptibility to Electromagnetic Transmissions

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

WEEE Compliance

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

Thermo Fisher Scientific has contracted with one or more recycling or disposal companies in each European Union (EU) Member State, and these companies should dispose of or recycle this product. See www.thermo.com/WEEERoHS for further information on Thermo Fisher Scientific's compliance with these Directives and the recyclers in your country.

WEEE Konformität

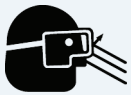
Dieses Produkt muss die EU Waste Electrical & Electronic Equipment (WEEE) Richtlinie 2002/96/EC erfüllen. Das Produkt ist durch folgendes Symbol gekennzeichnet:

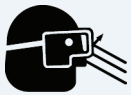
Thermo Fisher Scientific hat Vereinbarungen mit Verwertungs-/Entsorgungsfirmen in allen EU-Mitgliedsstaaten getroffen, damit dieses Produkt durch diese Firmen wiederverwertet oder entsorgt werden kann. Mehr Information über die Einhaltung dieser Anweisungen durch Thermo Fisher Scientific, über die Verwerter, und weitere Hinweise, die nützlich sind, um die Produkte zu identifizieren, die unter diese RoHS Anweisung fallen, finden sie unter www.thermo.com/WEEERoHS.

Conformité DEEE

Ce produit doit être conforme à la directive européenne (2002/96/EC) des Déchets d'Equipements Electriques et Electroniques (DEEE). Il est marqué par le symbole suivant:

Thermo Fisher Scientific s'est associé avec une ou plusieurs compagnies de recyclage dans chaque état membre de l'union européenne et ce produit devrait être collecté ou recyclé par celles-ci. Davantage d'informations sur la conformité de Thermo Fisher Scientific à ces directives, les recycleurs dans votre pays et les informations sur les produits Thermo Electron qui peuvent aider la détection des substances sujettes à la directive RoHS sont disponibles sur www.thermo.com/WEEERoHS.

CAUTION Symbol	CAUTION	VORSICHT	ATTENTION	PRECAUCION	AVVERTENZA
	**Electric Shock:** This instrument uses high voltages that can cause personal injury. Before servicing, shut down the instrument and disconnect the instrument from line power. Keep the top cover on while operating the instrument. 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 Wartungsarbeiten nicht mit abgenommenem Deckel. Nehmen Sie die Schutzabdeckung von Leiterplatten nicht ab.	**Choc électrique:** L'instrument utilise des tensions capables d'infliger des blessures corprelles. L'instrument doit être arrêté et débranché de la source de courant avant tout intervention. Ne pas utiliser l'instrument sans son couvercle. Ne pas elensver 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 debera apagarse y desconectarse de la línea de alimentacion eléctrica. No opere el instrumento sin sus cubiertas exteriores quitadas. No remueva las cubiertas protectoras de las tarjetas de circuito impreso.	**Shock da folgorazione.** L'apparecchio è alimentato da corrente ad alta tensione che puo provocare lesioni fisiche. Prima di effettuare qualsiasi intervento di manutenzione occorre spegnere ed isolare l'apparecchio dalla linea elettrica. Non attivare lo strumento senza lo schermo superiore. Non togliere i coperchi a protezione dalle schede di circuito stampato (PCB).
	**Chemical:** This instrument might contain hazardous chemicals. Wear gloves when handling toxic, carcinogenic, mutagenic, or corrosive or irritant chemicals. Use approved containers and proper procedures to dispose waste oil.	**Chemikalien:** Dieses Gerät kann gefährliche Chemikalien enthalten. Tragen Sie Schutzhandschuhe beim Umgang mit toxischen, karzinogenen, mutagenen oder ätzenden/reizenden Chemikalien. Entsorgen Sie verbrauchtes Öl entsprechend den Vorschriften in den vorgeschriebenen Behältern.	**Chimique:** Des produits chemiques dangereux peuven se trouver dans l'instrument. Proted dos 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 quimicos peligrosos. Utilice guantes al manejar productos quimicos tóxicos, carcinogenos, mutagenos 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 aprovo e seguire la procedura indicata per lo smaltimento dei residui di olio.
	**Heat:** Before servicing the instrument, allow any heated components to cool.	**Hitze:** Warten Sie erhitzte Komponenten erst nachdem diese sich abgekühlt haben.	**Haute Temperature:** Permettre aux composants chauffés de refroidir avant tout intervention.	**Altas temperaturas:** Permita que lop componentes se enfríen, ante de efectuar servicio de mantenimiento.	**Calore.** Attendere che i componenti riscaldati si raffreddino prima di effetturare l'intervento di manutenzione.
	**Fire:** Use care when operating the system in the presence of flammable gases.	**Feuer:** Beachten Sie die einschlägigen VorsichtsmaBnahmen, 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:** Dex projections chimiques, liquides, ou solides peuvent être dangereuses pour les yeux. Porter des lunettes de protection lors de toute manipulationde produit chimique ou pour toute intervention sur l'instrument.	**Peligro par los ojos:** Las salicaduras de productos químicos o particulas que salten bruscamente pueden causar lesiones en los ojos. Utilice anteojos protectores al mnipular 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 appears on the instrument to refer the user to instructions in this manual.	**Allgemeine Gefahr:** Es besteht eine weitere Gefahr, die nicht in den vorstehenden Kategorien beschrieben ist. Dieses Symbol wird im Handbuch auBerdem dazu verwendet, um den Benutzer auf Anweisungen hinzuweisen.	**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 categorias anteriores. Este simbolo también se utiliza en el instrumento par 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 questionable, contact your local Technical Support organization for Thermo Fisher Scientific 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 Fisher Scientific 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 Fisher Scientific 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 Fisher Scientific 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 Fisher Scientific San Jose.

CAUTION Symbol	CAUTION	危険警告	危險警告
	**Electric Shock:** This instrument uses high voltages that can cause personal injury. Before servicing, shut down the instrument and disconnect the instrument from line power. Keep the top cover on while operating the instrument. 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 計測器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儀器。請勿拆除PCB保護蓋。
	**Chemical:** This instrument might contain hazardous chemicals. Wear gloves when handling toxic, carcinogenic, mutagenic, or corrosive or irritant chemicals. Use approved containers and proper procedures to dispose 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:** Before servicing the instrument, allow any heated components to cool.	**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。	高温：請先等高温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 appears 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 questionable, contact your local Technical Support organization for Thermo Fisher Scientific 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。

Contents

Preface

About This Guide

This guide describes the modes of operation and principle hardware components of your LCQ Fleet system. In addition, this manual provides instructions for cleaning and maintaining your LCQ Fleet MS detector. The LCQ Fleet represents the latest refinement in the LCQ series of Thermo Scientific MS instruments for full-scan MS^n performance.

Related Documentation

In addition to this guide, Thermo Scientific provides the following documents for the LCQ Fleet MS detector:

- *LCQ Fleet Preinstallation Requirements Guide*
- *LCQ Fleet Getting Connected Guide*
- *LCQ Fleet Getting Started Guide*
- *Ion Max and Ion Max-S API Ion Source Hardware Manual*

The instrument control software also provides online Help.

Safety and Special Notices

Make sure you follow the precautionary statements presented in this guide. The safety and other special notices appear in boxes.

Safety and special notices include the following:

CAUTION Highlights hazards to humans, property, or the environment. Each CAUTION notice is accompanied by an appropriate CAUTION symbol.

IMPORTANT Highlights information necessary to prevent damage to software, loss of data, or invalid test results; or may contain information that is critical for optimal performance of the system.

Note Highlights information of general interest.

Tip Helpful information that can make a task easier.

Contacting Us

There are several ways to contact Thermo Scientific.

Assistance

For new product updates, technical support, and ordering information, contact us in one of the following ways:

Visit Thermo Scientific on the Web

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Contact Technical Support

Phone: 1-800-685-9535
Fax: 1-561-688-8736
E-mail: TechSupport.C+MS@thermofisher.com
Knowledge base: http://www.thermokb.com

Find software updates and utilities to download at http://mssupport.thermo.com.

Contact Customer Service

For ordering information in the U.S. and Canada:
Phone: 1-800-532-4752
Fax: 1-561-688-8731
Web site: www.thermo.com/finnigan

Changes to the Manual and Online Help

To suggest changes to this guide or to the online Help, use one of the following:

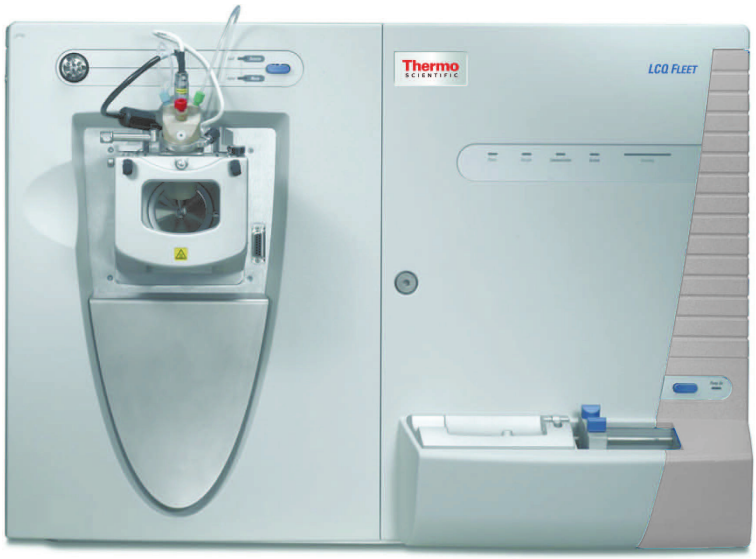
- Fill out a reader survey online at www.thermo.com/lcms-techpubs.
- Send an e-mail message to the Technical Publications Editor at techpubs.finnigan-lcms@thermofisher.com.

Introduction

Welcome to the LCQ™ Fleet MS detector. The LCQ Fleet is a member of the Thermo Scientific family of mass spectrometers.

The LCQ Fleet MS detector, shown in Figure 1, is a 3D quadrupole ion trap mass spectrometer that includes a syringe pump, a divert/inject valve, and the Ion Max-S API ion source.

Figure 1. LCQ Fleet MS detector



This chapter provides an introduction to the LCQ Fleet MS detector and contains the following sections:

Overview

In a typical LC/MS analysis, the liquid chromatograph (LC) portion of the system separates a mixture into its chemical components that the mass spectrometer detects and identifies by the mass spectrometer. The LC pump produces a solvent stream (the mobile phase) that passes through an LC column (containing the stationary phase) under high pressure. An autosampler introduces a measured quantity of sample into this solvent stream. As the solvent stream passes through the LC column, the sample separates into its chemical components. The rate at which the components of the sample elute from the column depends on their relative affinities to the mobile phase and the solid particles that make up the column packing. As the separated chemical components exit the LC column, they pass through a transfer line and enter the MS detector where they are ionized and analyzed. As the MS detector analyzes the ionized components and determines their mass-to-charge *m/z* ratios, it sends a data stream to the data system computer. In addition to supplying information about the mass-to-charge ratios of ionized compounds, the LCQ Fleet MS detector can also supply structural information by performing MS^n experiments.

With the LCQ Fleet MS detector, you have two additional ways to introduce a sample into the MS detector: infusion and flow injection. To introduce a sample by infusion, you connect the built-in syringe pump directly to the API source of the MS detector. To introduce a sample by flow injection, you connect a sample loop, a syringe fitting, and an LC pump to the divert/inject valve. After you fill the sample loop with sample, you switch the position of the divert/inject valve, which places the contents of the sample loop in the path of the solvent flow produced by the LC pump.

The LCQ Fleet MS detector consists of an atmospheric pressure ionization (API) source, ion optics, a mass analyzer, and an ion detection system. The ion optics, mass analyzer, and 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 ion optics transmit the ions produced in the API source 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 set up data acquisition methods for the LCQ Fleet to analyze positively or negatively charged ions or to switch between these polarity modes during a single run.

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. An automatic gain control (AGC) controls the function of these lenses and sets them to transmit the optimum number of ions to the mass analyzer.

The mass analyzer measures the mass-to-charge ratios of the ions produced in the API source. Selected ions are ejected from the mass analyzer and reach the ion detection system where they produce a signal. The detection system electronics then amplify this signal for analysis by the LCQ Fleet 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 LCQ Fleet 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 LCQ Fleet 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, gives the user greater flexibility in the instrumentation for solving complex analytical problems.

Ion Polarity Modes

You can operate the LCQ Fleet in two ion polarity modes: positive or negative. The LCQ Fleet controls 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.

Ionization Techniques

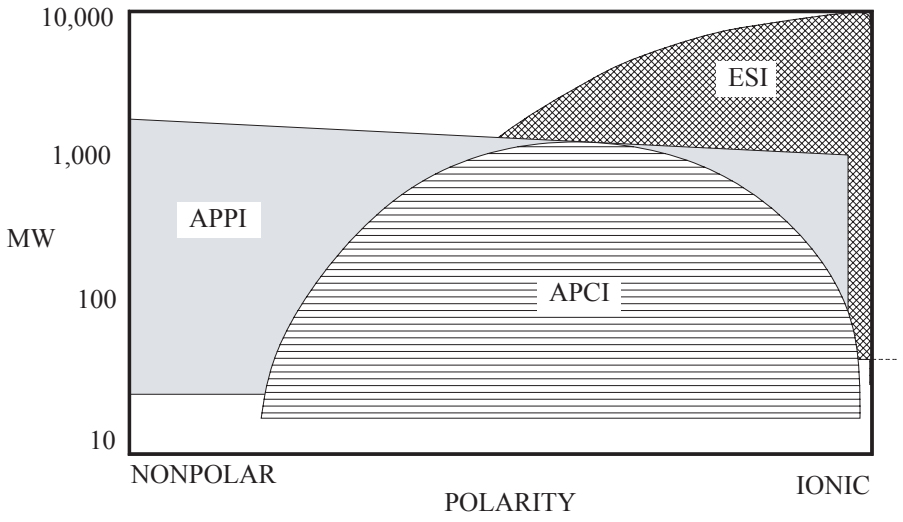
You can operate the LCQ Fleet using any of following four ionization techniques:

- Electrospray Ionization (ESI)
- Atmospheric Pressure Chemical Ionization (APCI)
- Atmospheric Pressure Photoionization (APPI)
- Nanospray Ionization (NSI)

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

Figure 2 shows the ranges of applicability (molecular weight as a function of polarity) of three of the ionization techniques being discussed: atmospheric pressure photoionization (APPI), atmospheric pressure chemical ionization (APCI), and electrospray ionization (ESI).

Figure 2. Molecular weight ranges of ionization techniques



Electrospray Ionization

The electrospray ionization (ESI) technique transforms ions in solution into ions in the gas phase[1]. ESI can be used to analyze many samples that previously were not suitable for mass analysis (for example, heat-labile compounds or high molecular weight compounds). ESI can be used to analyze 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 masses that can be analyzed by the LCQ Fleet is greater than 100000 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:

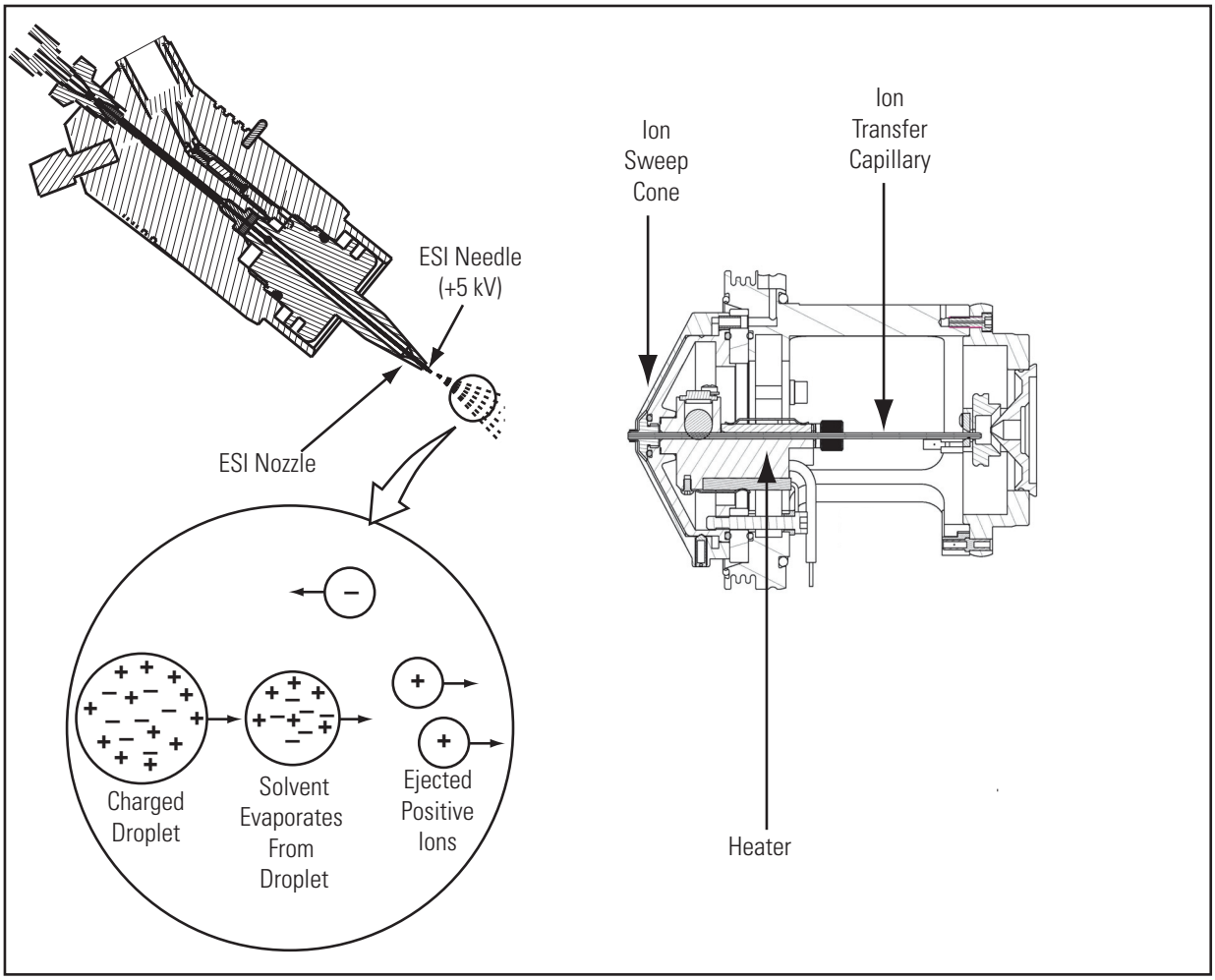
1. The sample solution enters the ESI needle, to which a high voltage is applied.
2. The ESI needle sprays the sample solution into a fine mist of droplets that are electrically charged at their surface.
3. The electrical charge density at the surface of the droplets increases as solvent evaporates from the droplets.

[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.

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. The electrostatic repulsion between the sample ions in these very small, highly-charged droplets causes the sample ions to be ejected into the gas phase.
6. The sample ions pass through an ion transfer capillary, enter the MS detector and are analyzed.

In the LCQ Fleet the ESI needle is 60 degrees 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 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 3. ESI process in the positive ion polarity mode



You can use the ESI probe in either positive or negative ion polarity mode.The polarity of the preformed ions in solution determines the ion polarity mode of choice; that is, 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.) With 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 (CH_3OH), acetonitrile CH_3CN), and isopropyl alcohol [$(CH_3)_2CHOH$], 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 (TEA), are also good for ESI. 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.

To ensure a good electrospray:

- 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 LCQ Fleet, the sample tube in the APCI nozzle is 60 degrees 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 include:

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

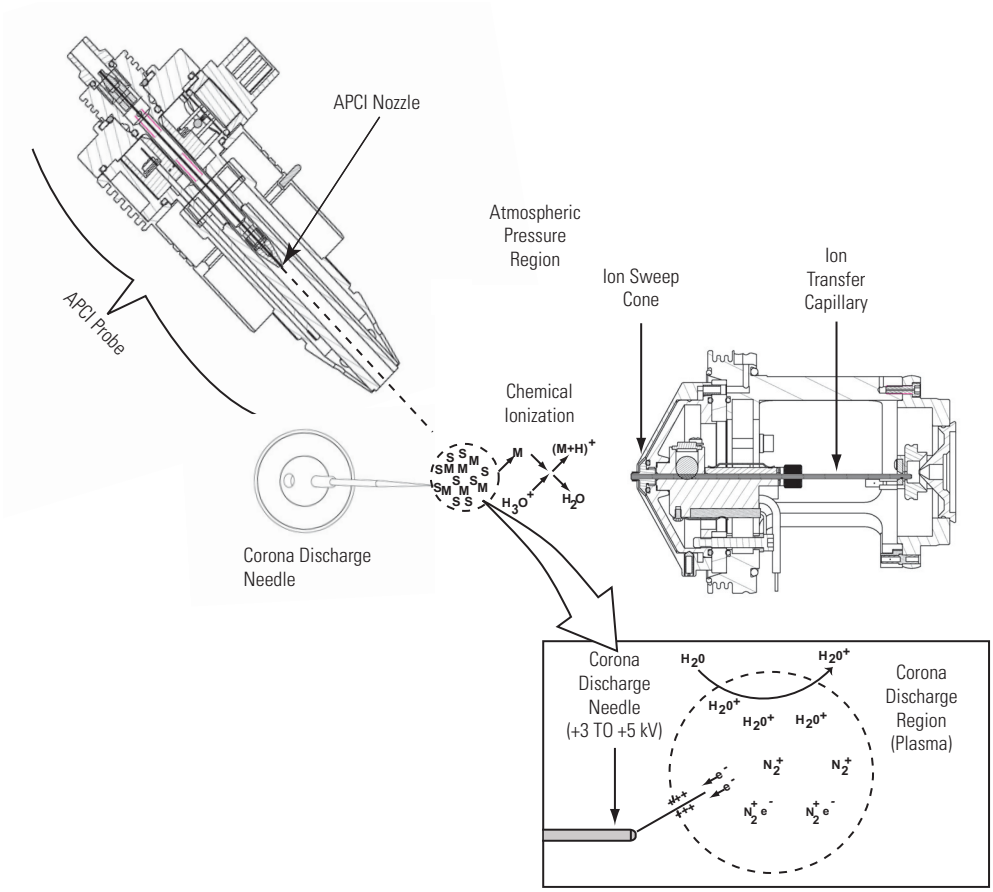
$$H_3O^+ + M \rightarrow (M+H)^+ + H_2O$$

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

APCI is used to analyze small molecules with molecular masses up to 2000 u. APCI is not affected by minor changes in most variables, such as changes in buffer or buffer strength.

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

Figure 4. APCI process in the positive ion polarity mode



You can use APCI in the positive-ion 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. Exceptions to this general rule are molecules with acidic sites such as carboxylic acids and acid alcohols, which produce more negative ions than positive ions.

While, 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 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 nitrogen in the 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 versus background. See Figure 5 and Figure 6.

Figure 5. Energetics of photoionization

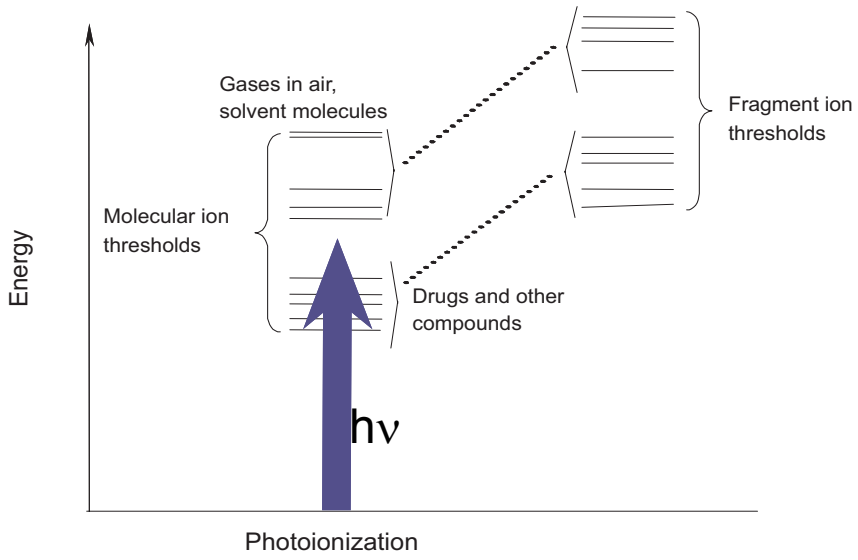
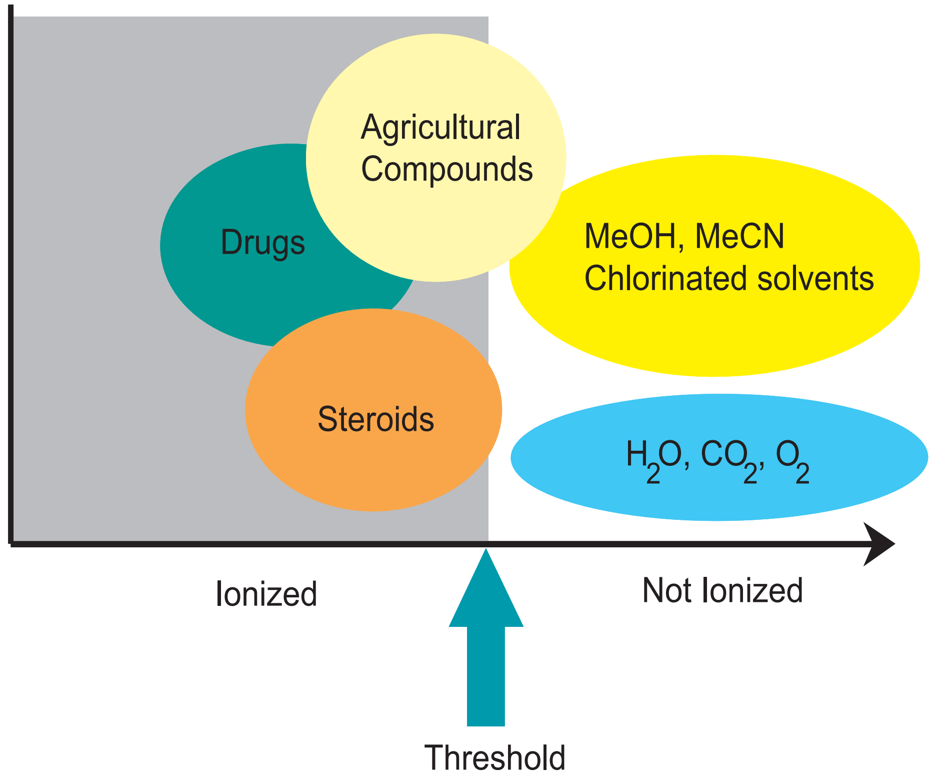


Figure 6. Selective photoionization



The light source is a krypton lamp that 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. The ionization potentials of typical compounds and solvents are listed below. Compounds and solvents with an ionization potential below 10 eV appear in red.

Compound Ionization Potentials (IP)		Solvent Ionization Potentials (IP)	
Anthracene	7.4 eV	Toluene	8.82 eV
Fluoranthene	7.8 eV	Acetone	9.7- eV
Caffeine	8.0 eV		
4-Nitrotoluene	9.5 eV		
10 eV - - - - - - - - - - - - - - - - - -			
		Methanol	10.85 eV
		Acetonitrile	12.19 eV
		Water	12.51 eV

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 minutes. 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 your NSI source.

Scan Power and Scan Modes

Ions produced in the ion source are often referred to as parent ions. To produce a mass spectrum, the mass analyzer varies its DC and RF voltages to sequentially eject ions from the trap based on their *m/z* values. Alternatively, by varying the RF voltages of the mass analyzer, the LCQ Fleet can first eject all ions, except for several selected ***parent ions***, and then collide these ions with the helium that is present in the mass analyzer. This helium is known as buffer gas. The collisions can cause the selected parent ions, also known as ***precursor ions***, to fragment into ***product ions***, which can then be sequentially ejected from the trap based on their *m/z* values to produce a mass spectrum.

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. The LCQ Fleet supports scan powers of n = 1 to n = 10. As you raise the scan power, you can obtain more structural information about the analyte.

The scan powers supported by the LCQ Fleet 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 mass spectrometry (MS) scan mode corresponds to a single stage of mass analysis (that is, a scan power of n = 1). The MS scan mode only involves parent ions, and no fragmentation of the parent ions occurs. The MS scan mode can be a full scan experiment or a selected ion monitoring (SIM) experiment (see "Selected Ion Monitoring" on page 13).

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 "Selected Reaction Monitoring" on page 14).

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 "Consecutive Reaction Monitoring" on page 14).

Scan Types

You can operate the LCQ Fleet in the following scan types:

- Full Scan
- Selected Ion Monitoring (SIM)
- Selected Reaction Monitoring (SRM)
- Consecutive Reaction Monitoring (CRM)
- ZoomScan

Full Scan

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

A full scan provides more information about an analyte than does selected ion monitoring (SIM) or selected reaction monitoring (SRM). A full scan does not provide the sensitivity that the other scan types can achieve.

The full scan type includes the following:

- Single-Stage Full Scan
- Two-Stage Full Scan

Single-Stage Full Scan

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

Use single-stage full scan experiments 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 can use SIM or SRM for routine quantitative analysis of the compound.

Two-Stage Full Scan

The two-stage full scan has two stages of mass analysis (where n = 2 scan power). In the first stage, 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 and 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 gives you more information about a sample than does SRM but does not yield the speed that SRM can achieve. With a two-stage full scan, you spend more time monitoring the product ions than you do with SRM. Thus, the two-stage full scan provides greater information but at a lower speed than SRM does.

To use the SRM scan you must know which parent and product reaction ions to observe. To obtain this information you could use a one-stage full scan to determine the parent mass spectrum and a two-stage full scan to determine the product mass spectrum for the parent ions of interest. For subsequent routine quantitative analysis you would use an SRM scan type based on the one-stage and two-stage full scan results.

Selected Ion Monitoring

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

Use SIM experiments to detect small quantities of a target compound in a complex mixture when you know the mass spectrum of the target compound. SIM is useful in trace analysis and in the rapid screening of a large number of samples for a target compound.

Because a SIM scan monitors only a few ions, SIM provides lower detection limits and greater speed than a single-stage full scan analysis. 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 it only monitors a few ions of interest; 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 target compound specificity. This is because SIM analysis only monitors particular ions. Thus, any compound that produces the ion or ions being monitored would appear to be the target compound. Verify that the ions being monitored with SIM are from the target compound and nothing else; otherwise you can obtain false positive results.

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. The parent ions are then 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. The selected ions are then sequentially scanned out of the mass analyzer to produce an SRM product ion mass spectrum.

Like SIM, SRM allows for 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 form a parent ion of the same mass-to-charge ratio as the selected parent ion from the target compound. The compound 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), that monitors a multistep reaction path. 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 then 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 producing one or more new product ions.

In the third stage of mass analysis, the new product ions are stored in the mass analyzer. This process 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. The selected ions are then 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 many fragmentation pathways are available to the ion.

ZoomScan

Determining of the mass of an ion from its mass-to-charge ratio can be complicated if the charge state of the ion is unknown. ZoomScan is a high resolution MS scan in which the LCQ Fleet performs a high resolution scan to determine the charge state and molecular mass of an ion. The LCQ Fleet 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 that you want to examine.

Data Types

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

- Profile Data
- Centroid Data

Profile Data

With profile data 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

With centroid data 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. The disk space requirements for centroid data are about one-tenth of what is required for profile data. Consequently, data processing for centroid data is faster than that for profile data.

Experiment Types

You can perform several types of experiments with the LCQ Fleet. The experiments are grouped into the following categories:

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

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

Note Procedures for these experiments are beyond the scope of this manual. If you need more information, refer to the 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 that you can get started with a General MS or MS^n experiment.

In a General MS quantitation experiment, you must specify the mass range of your analyte(s) of interest, a parent (precursor ion) that fragments into distinctive product ions, and the mass-to-charge ratios of all the parent ions of interest. The LCQ Fleet 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 select the parent ion(s) for which you want data in the Set Parent List dialog box. The LCQ Fleet then collects distinct qualitative information for structural analysis or for spectral reference.

The LCQ Fleet can generate reproducible, product-specific spectra, even from laboratory to laboratory. Consequently, you can use reference spectra that are generated with the LCQ Fleet to confirm structures of compounds generated with other LCQ Fleet systems.

Data-Dependent Experiments

Use Data-Dependent experiments for the qualitative analysis of unknown compounds for structure elucidation or confirmation. The LCQ Fleet 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 LCQ Fleet automatically select the ions for fragmentation. The LCQ Fleet 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 about how the experiment should best proceed, as long as you specify that one or more scan events of an experiment segment are to be run as Data-Dependent. The LCQ Fleet then 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 LCQ Fleet can decide which parent ion to isolate, the charge state of the parent ion, and the molecular mass 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 a type of Data-Dependent experiment that provide methods for automatically interpreting MS^n data and arranging the data in easy-to-manipulate formats.

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 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 LCQ Fleet generates product spectra. Later, you decide if the information is useful. Parameters might include threshold values for the intensity of the MS or MS^n ion signal. Whatever threshold values you choose should isolate 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 need to specify a parent ion. The LCQ Fleet then collects full scan MS data, picks the most intense parent ion in the spectrum, and fragments 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 LCQ Fleet 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 LCQ Fleet determines a charge state equal to two, 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 and including *m/z* 1000 (or 2 × 500).

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).

  For example in the quality assurance process for aspirin, the LCQ Fleet can identify impurities of 0.1%.

- Identify metabolites in a complex mixture (Chromatographic Separation with Data-Dependent MS/MS).

  For example characteristic masses along the metabolic pathways of a drug can produce MS/MS spectra that are specific to the structure of the drug. These spectra are essential to metabolite identification.

- Build a custom library of composite MS^n spectra (Ion Tree).

  A Data-Dependent experiment can produce a composite spectrum of, for example, MS^2, MS^3, and MS^4 data. The LCQ Fleet 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

Use an Ion Mapping experiment 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 LCQ Fleet includes Ion Mapping templates in Instrument Setup.Use one of the following templates to start with an Ion Mapping experiment:

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

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

In a Total (or full scan) Ion Mapping experiment, product ion scans are produced for each parent ion, so you can determine which parent ions lost a particular fragment to yield a particular product ion. Furthermore, 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.

You can view the results of any of the Ion Mapping experiments in the Xcalibur Qual Browser window.

Ion Tree Experiments

In an Ion Tree experiment, the LCQ Fleet can collect MS^n data automatically. You can specify a particular parent ion for fragmentation or let the LCQ Fleet find the parent ions automatically and fragment them to any level between MS^2 and MS^{10}. The LCQ Fleet 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 to prioritize how the LCQ Fleet gathers information, Depth Focus or Breadth Focus.

- Depth Focus characterizes an ion by performing a series of MS^n-level fragmentations (for example, MS/MS, MS^3, MS^4, and so on) 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 three and a Maximum Breadth of two in an Ion Tree experiment, the following occurs:

1. With either Depth or Breadth Focus, the LCQ Fleet scans for parent ions (MS) over the specified mass range. The most intense ion of the MS spectrum is selected for fragmentation (MS/MS).
2. If you chose the Depth Focus, after the most intense ion of the MS spectrum is fragmented—producing an MS/MS spectrum—the LCQ Fleet 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 LCQ Fleet 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.
3. If you chose the Breadth Focus, after the most intense ion of the MS spectrum is fragmented—producing an MS/MS spectrum—the LCQ Fleet 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 (in this example, two). After the two most intense peaks on the MS level are fragmented, the LCQ Fleet 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.

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

Functional Description

This chapter describes the principal components of the LCQ Fleet LC/MS system and their respective functions.

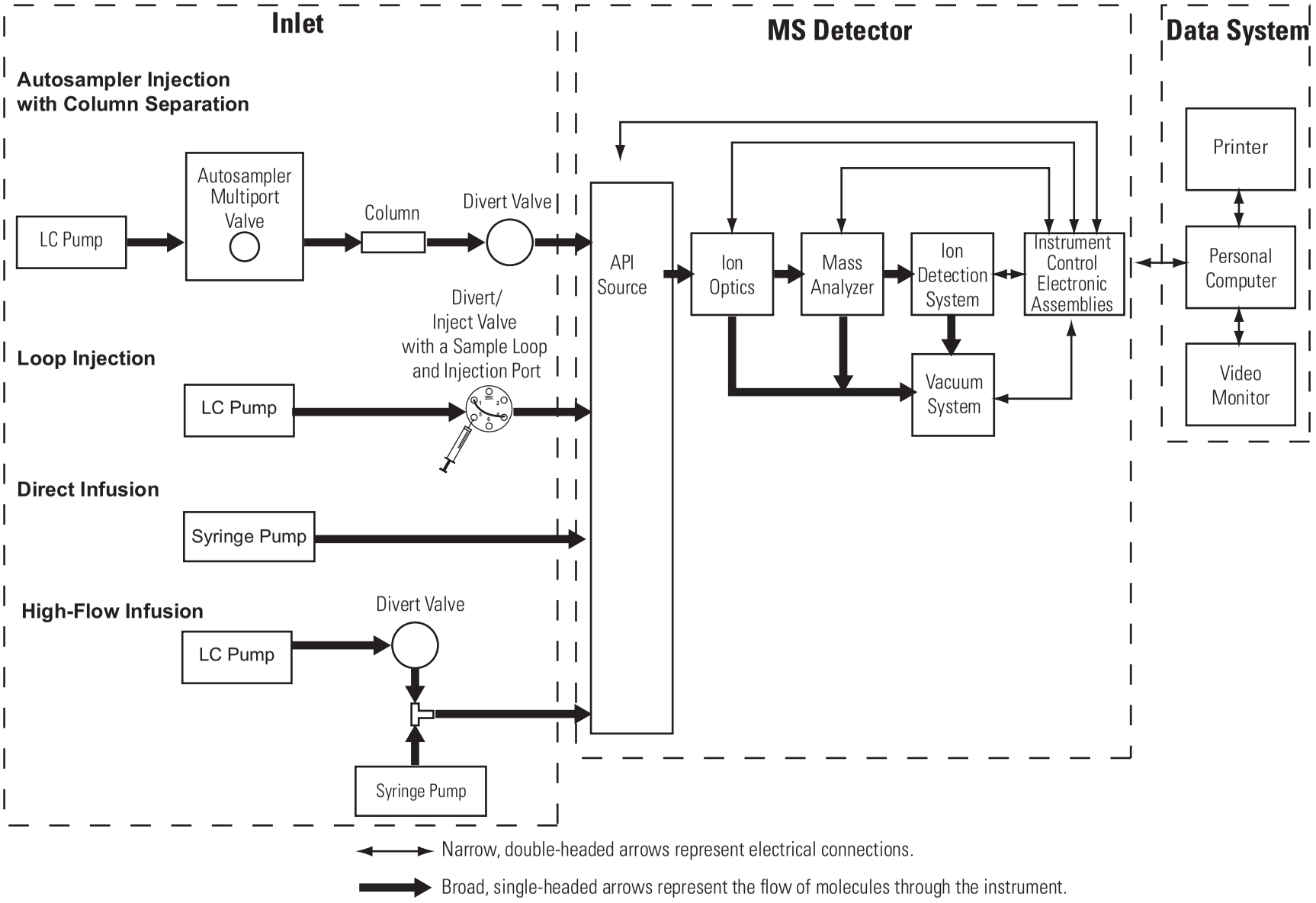
This chapter contains the following sections:

Figure 7 shows a functional block diagram of the LCQ Fleet system. A sample transfer line connects the liquid chromatograph (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 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 atmospheric ionization (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 an ion detection system that produces a current proportional to the number of ions detected. The current from the ion detection system is received and amplified by the LCQ Fleet electronics. This current is then passed on to the data system for further processing, storage, and display. The data system provides the primary LCQ Fleet user interface.

Figure 7. The LCQ Fleet system (functional block diagram)



Liquid Chromatography System

In general, a liquid chromatography system, used as an inlet for a mass spectrometer, consists of an autosampler, an analytical pump, and an LC column. Some autosamplers include a built-in column oven, and some LC systems contain an additional column heater device.

This section contains the following topics:

Autosampler

The autosampler is used to inject samples automatically into the mobile phase stream produced by the liquid chromatography pump. You can control the Thermo Scientific autosampler (Surveyor Autosampler or Accela Autosampler) Waters 2795 Separations module, and Agilent (1100) autosamplers directly from the Xcalibur data system. With an autosampler, you can automate your LC/MS analyses.

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

To control an autosampler from the Xcalibur data system, you must first add it to your instrument configuration. Refer to the online Help provided with the Xcalibur Instrument Configuration application for more information on configuring your autosampler.

After you add the autosampler to the instrument configuration, you can specify its injection parameters in the Xcalibur Instrument Setup application. Refer to the Xcalibur online Help for a description of the Instrument Setup application.

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

Liquid Chromatography Pump and Column

The high performance liquid chromatograph (LC), which consists of an LC pump and an LC column, 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.

You can control the Thermo Scientific (Surveyor MS Pump, Surveyor LC Pump Plus, or Accela Pump), and Agilent (1100) LCs (and the corresponding UV detectors) directly from the Xcalibur data system. Refer to the *LCQ Fleet Getting Connected* manual for information on connecting an LC to the LCQ Fleet MS detector.

To control the devices of your liquid chromatograph, you must first add them to your instrument configuration. Refer to the online Help provided with the Xcalibur Instrument Configuration application for more information on configuring these devices.

After you add an LC pump to your instrument configuration, you specify the chromatographic parameters in the Xcalibur Instrument Setup application. Refer to the Xcalibur online Help for a description of the Instrument Setup application.

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

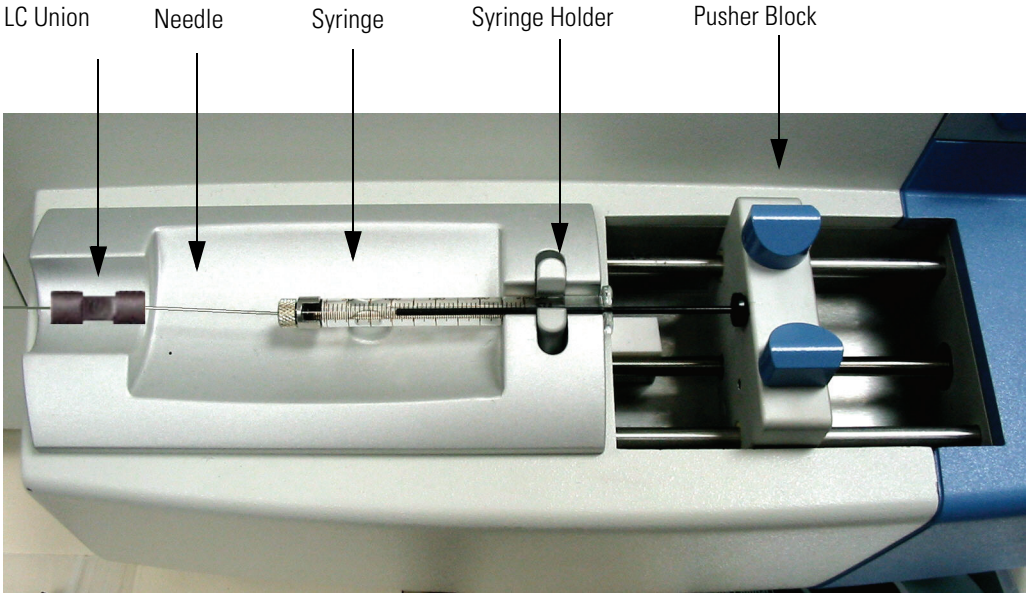
Syringe Pump

The LCQ Fleet includes an electronically controlled, integrated, syringe pump. The syringe pump delivers sample solution from the syringe into the API source. See Figure 8. When the syringe pump is operating, a motor drives a pusher block that depresses the plunger of the syringe at a rate (volume per minute) that is user adjustable. Liquid flows out of the syringe needle and into the sample transfer line as the plunger is depressed. A syringe holder keeps the syringe in place. Refer to the *LCQ Fleet Getting Started Guide* 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 (or by choosing **Start > All Programs > Xcalibur > LCQ Fleet Tune**). Refer to the Xcalibur online Help for instructions on operating the syringe pump from the data system.

The syringe pump light emitting diode (LED) is green whenever the syringe pump is pumping. The LED is off if the syringe pump is at the end of its travel.

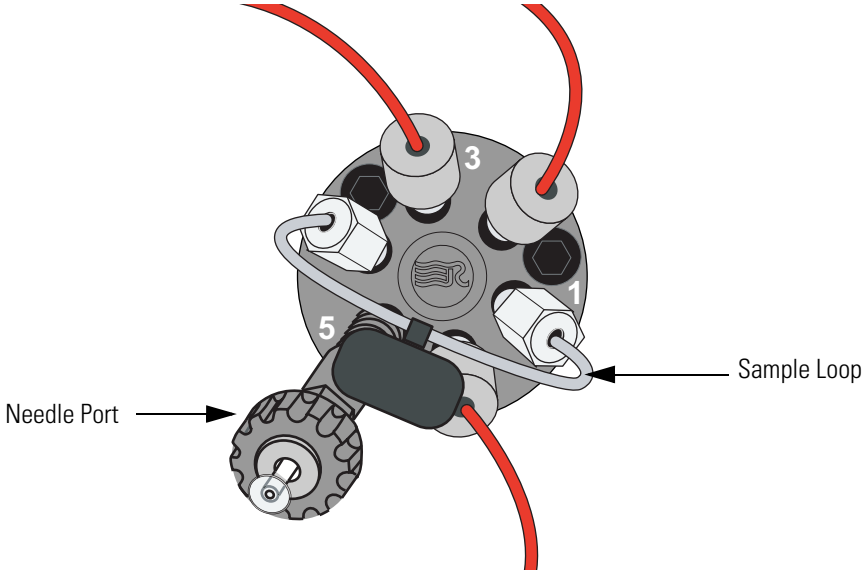
Figure 8. Syringe pump



Divert/Inject Valve

The divert/inject valve is located on the front of the LCQ Fleet to the left of the API source. See Figure 9.

Figure 9. Divert/inject valve set up for flow injection analyses



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 as a loop injector or a divert valve are provided in both the *LCQ Fleet Getting Connected Guide* and the *LCQ Fleet Getting Started Guide*.

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, located in the Tune Plus window, or the Divert Valve page, located in 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.

Mass Spectrometer (MS) Detector

The MS detector provides sample ionization and mass analysis of samples injected directly into the inject/divert valve or samples eluted from a liquid chromatograph. The LCQ Fleet MS detector uses a three-dimensional ion trap mass analyzer with an ion source external to the mass analyzer.

The primary components of the mass spectrometer are as follows:

- Manual Controls and LED Indicators
- API Source
- Ion Optics
- Mass Analyzer
- Ion Detection Systems
- Vacuum System and API Source Gas Hardware
- Cooling Fans
- Electronic Assemblies

Manual Controls and LED Indicators

The LCQ Fleet has the following LED indicators and manual controls:

- Front Panel LEDs
- Main Power Circuit Breaker Switch
- Electronics Service Switch
- Reset Button
- Divert/Valve LEDs and Push-Button
- Syringe Pump LED and On/Off Push Button

Front Panel LEDs

Five indicator LEDs (light-emitting diodes)—labeled Power, Vacuum, Communication, System, and Scanning— are located on the upper-right side of the MS detector as shown in Figure 10.

Figure 10. Front panel LEDs of the MS detector

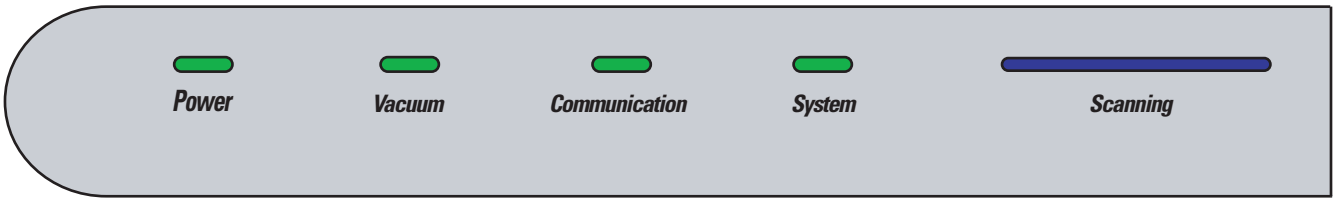


Table 1. LED indicators

State	Yellow	Green	Not Illuminated	Flashing Blue
Power LED	N/A	Power is being supplied to the vacuum system and electronic assemblies of the MS detector.	Power is not being supplied to the LCQ Fleet.	N/A
Vacuum LED	A vacuum sensor detects a fault and power is being applied to the LCQ Fleet components.	The vacuum protection circuitry indicates that the vacuum is within the allowable operating range.	High voltage is not being applied to the LCQ Fleet components.	N/A
Communication LED	The MS detector and the data system are trying to establish a communication link.	The data system is communicating with the MS detector.	Power is not being supplied to the LCQ Fleet.	N/A
System LED	The API interlock is open (that is, high voltage is not supplied to the API source, mass analyzer, and ion detection system) and the MS detector power is on.	The MS detector is on and high voltage is being supplied to the API source, mass analyzer, and ion detection system.	Power is not being supplied to the LCQ Fleet.	N/A
Scanning LED	N/A	N/A	The MS detector is not scanning ions.	The MS detector is on and scanning ions.

Main Power Circuit Breaker Switch

The main power circuit breaker switch (labeled Main Power) is located on the power panel, which is located on the lower portion of the right side panel of the MS detector. See Figure 11. In the Off (O) position, the circuit breaker removes all power to the MS detector, including the external forepump. 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.

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

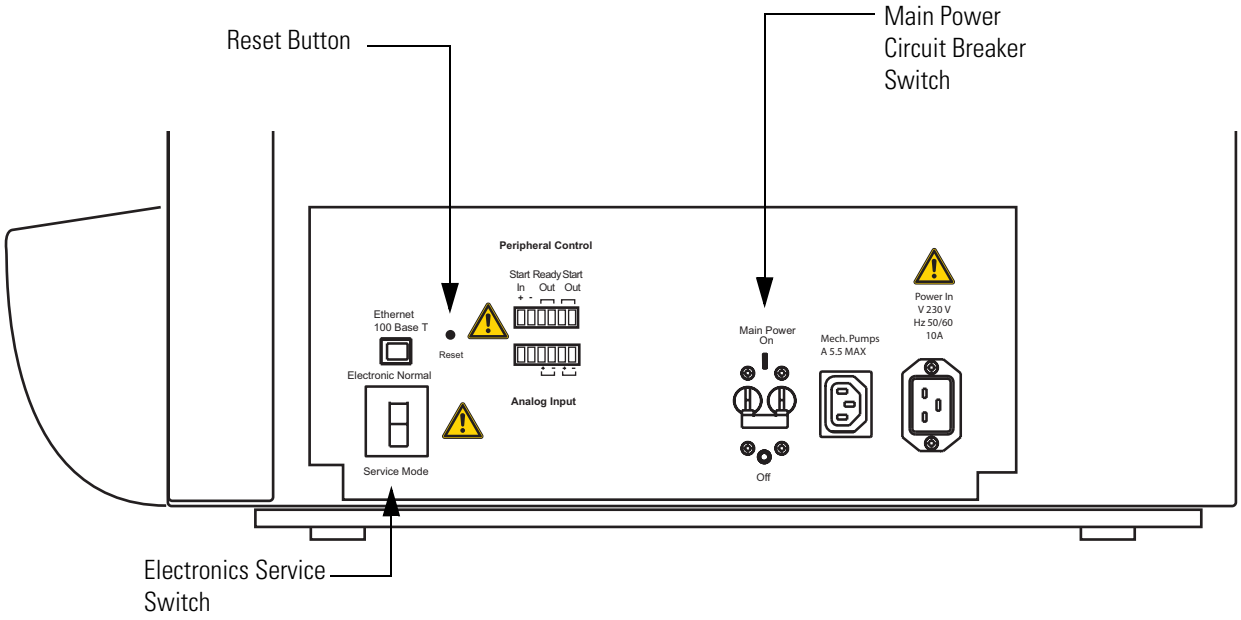
Electronics Service Switch

The electronics service switch is located on the power panel as shown in Figure 11. In the Service position, the switch removes power to all components of the MS detector other than the vacuum system, which includes both the forepump and turbomolecular pump. In the Electronics Normal position, power is supplied to all components of the MS detector.

Reset Button

The reset button is also located on the power panel. When you briefly press the reset button, the LCQ Fleet software is reloaded from the data system. See "Resetting the MS Detector" on page 117 in Chapter 5 of this manual for information on resetting the MS detector.

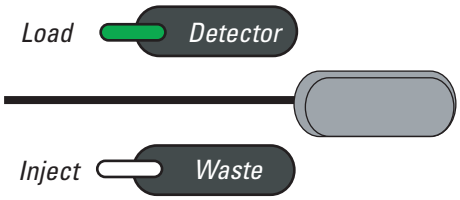
Figure 11. Power panel



Divert/Valve LEDs and Push-Button

The push-button switch located on the front panel above the divert/inject valve toggles the position of the two-position valve. LEDs to the left of the button indicate the position of the valve as shown in Figure 12.

Figure 12. Divert/inject valve button and LEDs



When the divert/inject valve is set up for loop injections (flow injection analysis, FIA), pressing the divert/inject valve button toggles the valve between the load and inject modes. The Load and Inject LEDs indicate the position of the valve.

When the divert/inject valve is set up for divert valve operation, pressing the divert/inject valve button toggles the LC flow between the MS detector and the waste container. The Detector and Waste LEDs indicate the position of the valve.

Syringe Pump LED and On/Off Push Button

The blue push-button switch located on the front panel above the syringe pump toggles the syringe pump on and off. An LED above the button indicates whether the pump is on or off.

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 the electrospray ionization (ESI), atmospheric pressure chemical ionization (APCI), atmospheric pressure photoionization (APPI), or nanospray ionization (NSI) techniques.

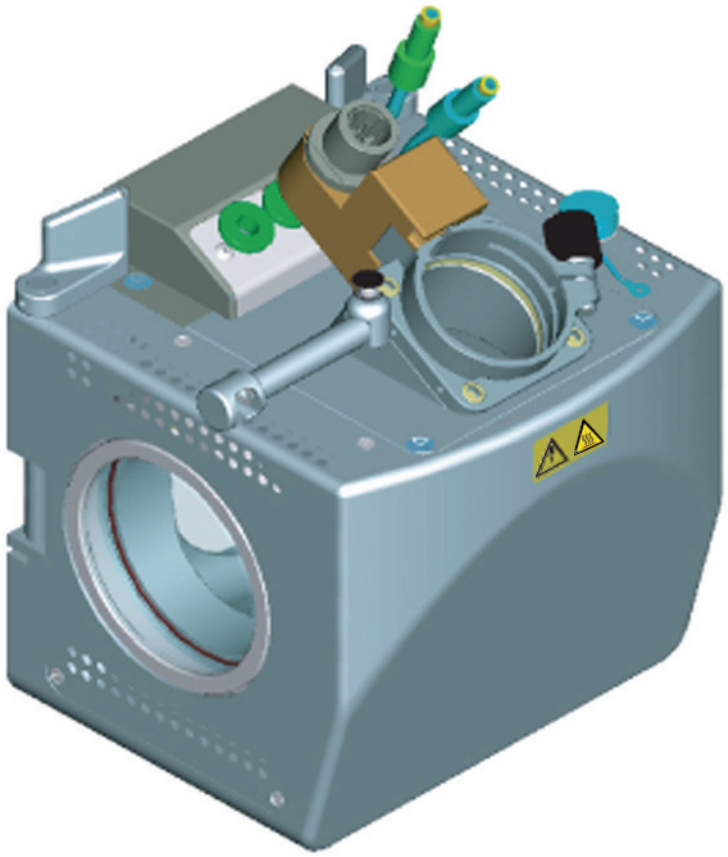
The API source consists of the following:

- Ion Max-S Ion Source
- Ion Source Interface

Ion Max-S Ion Source

The Ion Max-S™ ion source, shown in Figure 13, is the part of the API source that is at atmospheric pressure. The Ion Max-S™ ion source can be configured to operate in any of several API modes, including electrospray ionization (ESI), atmospheric pressure chemical ionization (APCI) and atmospheric pressure photoionization (APPI). The ion optics transmit the ions produced in the API source into the mass analyzer, where they are separated according to their mass-to-charge ratios.

Figure 13. Ion Max-S ion source



The Ion Max-S ion source housing enables you to quickly switch between ionization modes without the need for specialized tools. Ventilation in the ion source housing keeps the housing cool and easy to handle. The ion source is kept at atmospheric pressure. The probe mounting angle is fixed at the optimum angle for signal intensity and ion source robustness. The probe position in the Z dimension is adjustable to allow for further optimization of signal intensity. A view port, which enables visual control of probe positioning and monitoring during operation, and facilitates the addition of accessories, is located at the side of the ion source housing.

The ion source lifetime is excellent due to several special features. The drain size and angle prevent 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 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-S ion source has 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-S ion source, refer to the *Ion Max and Ion Max-S API Source Manual*.

Ion Source Interface

The ion source interface consists of the components of the API source that are held under a vacuum (except for the atmospheric pressure side of the ion sweep cone). The ion source interface includes an ion sweep cone, vent prevent ball, ion transfer capillary, two cartridge heaters, heater block, platinum probe sensor, tube lens, and skimmer. See Figure 14 and Figure 15.

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

The ***ion transfer capillary*** assists in desolvating ions that are produced by ESI, APCI, NSI, or APPI. This capillary is a metal, 4-in. long cylindrical tube. 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. 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 system electronics includes an over-temperature/under-temperature circuit and a voltage monitor circuit to protect the heaters. The voltage monitoring circuit detects shorting failures. The over-temperature circuit operates as a thermal limit switch to prevent the heater from going above a preset maximum temperature. The under-temperature feature protects against false low temperature readings. These could occur due to faults in the platinum probe temperature sensor that prevent it from sensing the preset maximum temperature. Such false low temperature readings could cause the heater to run at its maximum setting and cause damage to the capillary.

Ions from the ion transfer capillary enter the ***tube lens***. The tube lens has a mass dependent potential applied to it that focuses the ions towards the opening of the skimmer. When you tune the LCQ Fleet, 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 RF lens. The skimmer acts as a vacuum baffle between the higher pressure ion source interface region and the lower pressure Q00 region of the vacuum manifold.

The ion source interface is enclosed in a vacuum chamber that is evacuated by the forepump (also known as s a rotary-vane pump or mechanical pump).

Figure 14. Cross sectional view of the ion source interface and Q00/L0RF lens

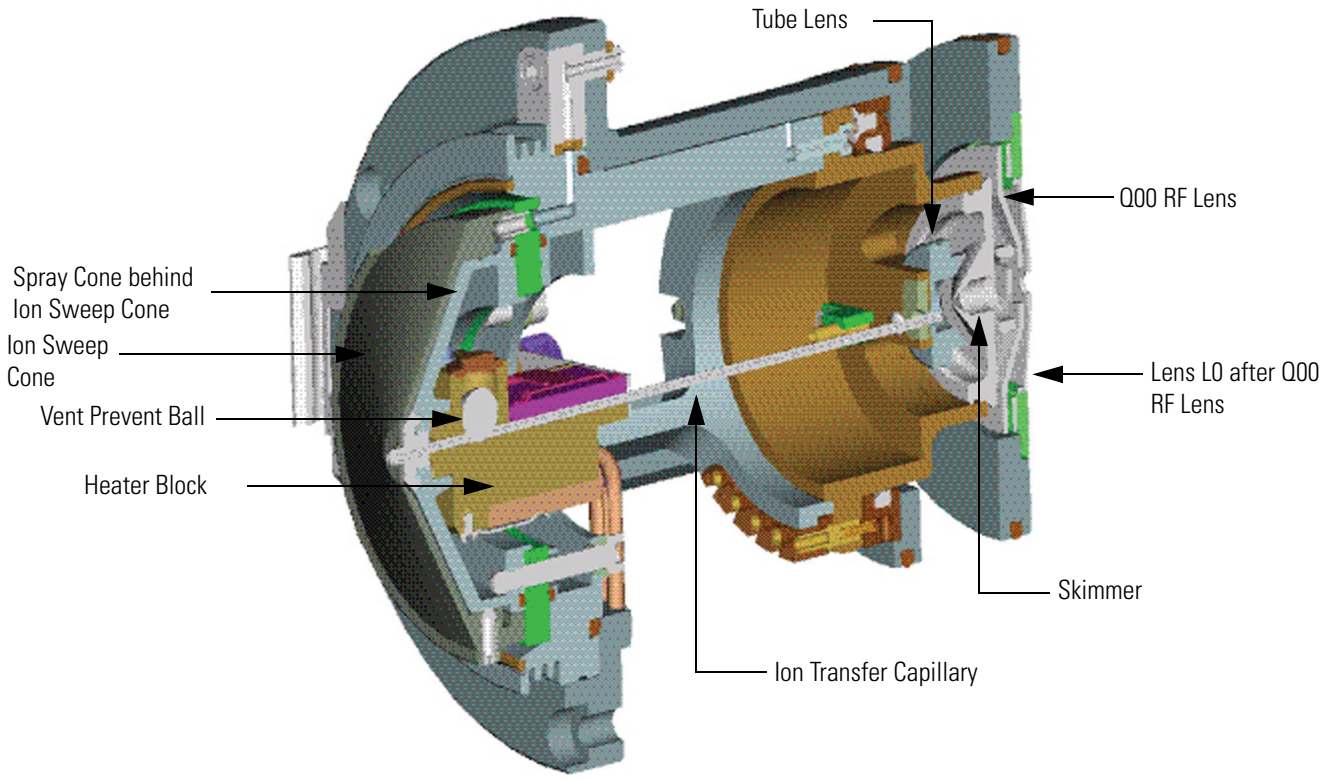
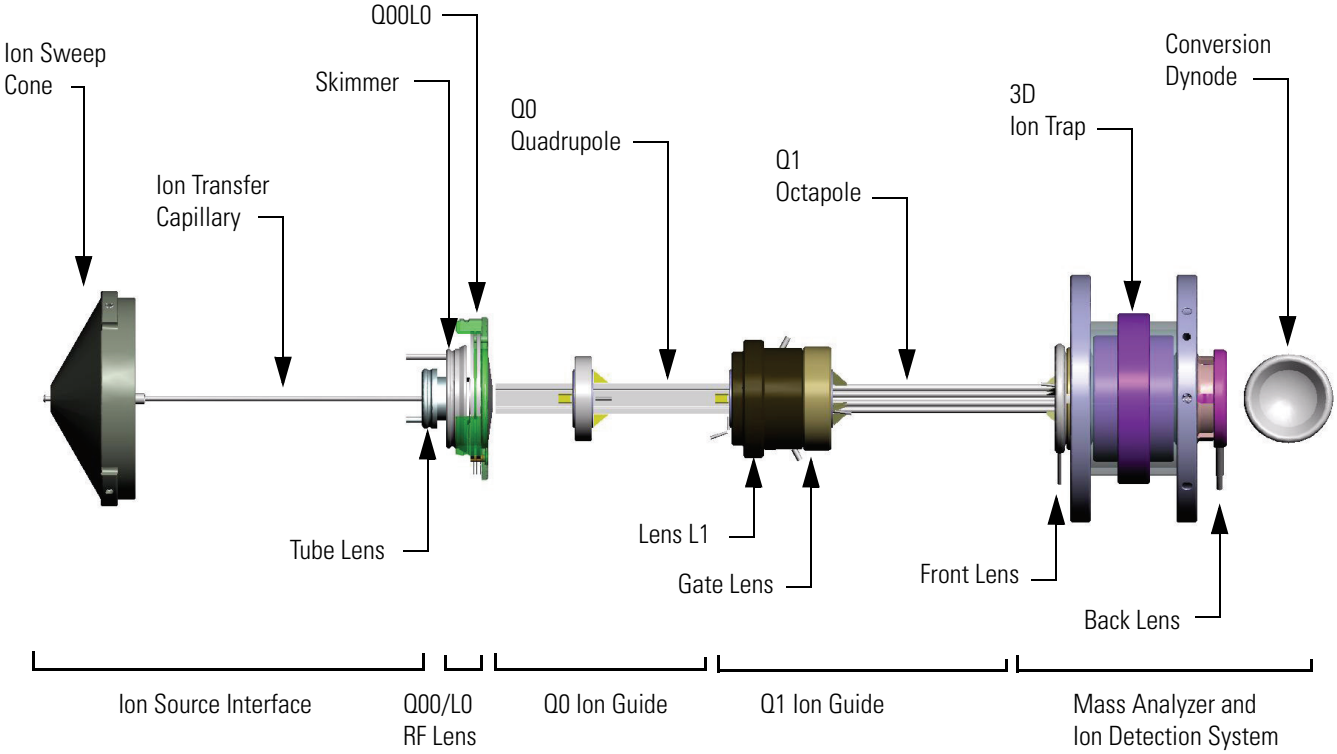


Figure 15. Internal (under vacuum) components of the MS detector



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 the following:

- Q00/L0 RF Lens
- Q0 Ion Guide
- Q1 Ion Guide

Q00/L0 RF Lens

The Q00/L0 RF lens is located closest to the API source. The Q00/L0 RF lens includes the Q00 RF lens and L0 lens. See Figure 14 and Figure 15.

The Q00 RF lens is a square array of square-profile segments that act as an ion focusing device. Any RF voltage that is applied to the optics produces an electric field that focuses the ions along the axis of the Q00 RF lens. A dc voltage offset from ground that is applied to the Q00 RF lens—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 increases 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 disk with a circular hole in the center through which the ion beam can pass. An electrical 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 RF lens and the Q0 ion guide. The Q00 RF lens chamber of the vacuum manifold is evacuated 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 RF lens to the Q1 ion guide. The Q0 ion guide includes the Q0 quadrupole and lens L1. See Figure 15.

The Q0 quadrupole is a square array of square-profile rods that act as an ion transmission device similar to the Q00 RF lens. An RF voltage that is applied to the rods produces 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 the Q00 RF lens. Q0 must be at a lower potential than the Q00 RF lens.

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 ±125 V. Lens L1 also acts as a vacuum baffle between the Q0 ion guide chamber and the mass analyzer chamber. The interstage inlet of the turbomolecular pump evacuates the Q0 ion guide chamber.

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 15.

The Q1 octapole is an octagonal array of round-profile rods that act as an ion transmission device similar to the Q00 RF lens and Q0. An RF voltage that is applied to the rods produces 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 starts and stops the injection of ions into the mass analyzer.

The front lens focuses the ions before entering the trap.

Mass Analyzer

The mass analyzer is the site of mass analysis (that is, ion storage, ion isolation, collision induced dissociation, and ion scanout). This topic describes the following:

- Components of the Mass Analyzer
- Main RF Voltage Applied to the Mass Analyzer Ring Electrode
- Voltages Applied to the Mass Analyzer End Caps
- Helium Gas in the Mass Analyzer Cavity
- Operation of the Mass Analyzer During Mass Analysis

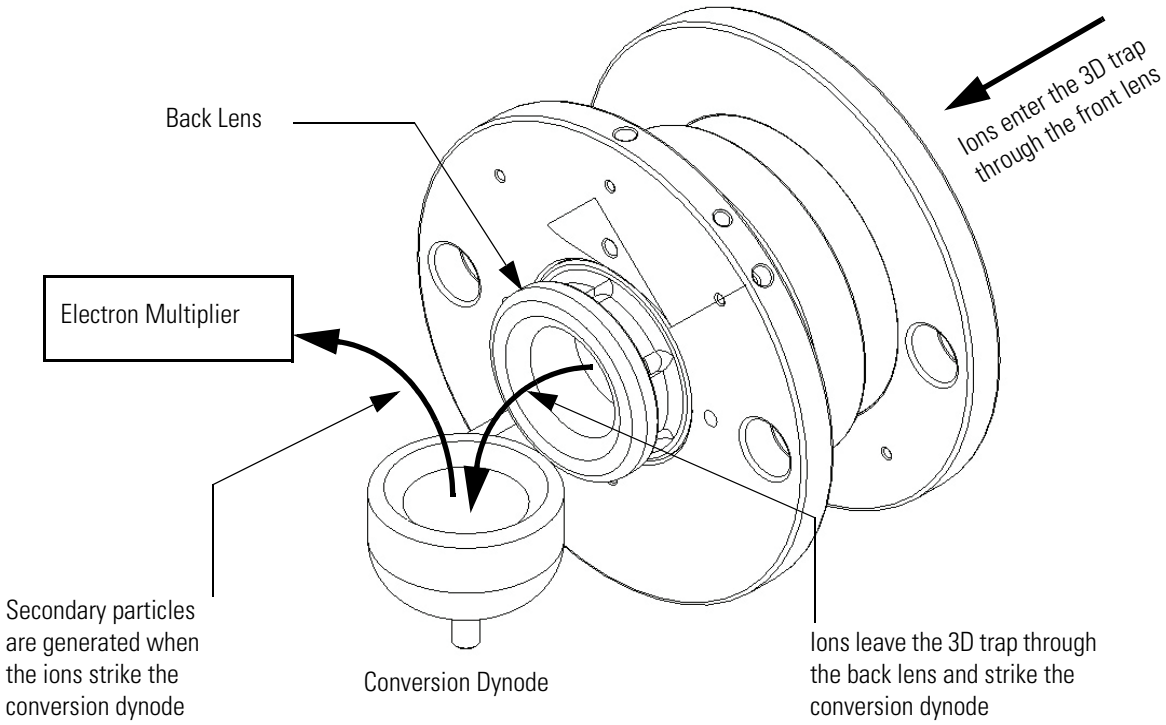
Components of the Mass Analyzer

The mass analyzer consists of an entrance endcap electrode, ring electrode, and the exit endcap electrode (see Figure 15). The entrance endcap electrode and exit endcap electrodes are metal disks with circular holes in their centers through which the ion beam can pass. The inner surfaces of these electrodes have a complex shape. The electrodes form a cavity in which mass analysis occurs.

The entrance endcap electrode is the electrode that is closest to the ion optics, and the exit endcap electrode is the electrode that is closest to the ion detection system. Both endcap electrodes have a small hole in their centers to permit the passage of ions into and out of the mass analyzer cavity. The ring electrode is located between the endcap electrodes. Ions produced in the API source enter the mass analyzer cavity through the entrance endcap electrode. Ions are ejected through either endcap electrode during mass analysis. The conversion dynode accelerates ions ejected from the exit endcap towards the ion detection system. The potential of the conversion dynode relative to the exit endcap, which is at ground potential, creates the accelerating potential. Helium damping gas enters the mass analyzer cavity through a nipple on the entrance endcap electrode.

Two quartz space rings separate the entrance endcap electrode, exit endcap electrode, and ring electrode. The spacer rings position the electrodes at the proper distance apart and also serve as electrical insulators. Two nonconducting analyzer posts pass through both endcap electrodes and screw into the analyzer mount (also nonconducting). A spring washer and analyzer nut on the end of each post apply a force to the exit endcap electrode that holds the electrodes and spacers in place.

Figure 16. The 3D ion trap assembly



Main RF Voltage Applied to the Mass Analyzer Ring Electrode

The RF voltage is applied only to the ring electrode (see Figure 16) and is of constant frequency (825 kHz) and of variable amplitude (0 to 10000 V zero-to-peak). Because the frequency of this RF 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 ring electrode produces a three-dimensional quadrupole field within the mass analyzer cavity. This time-varying field drives ionic motion in the axial radial direction. Ionic motion must be stable in both directions 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 axial direction. The ions are ejected from holes in the end caps and go to the dynode (Figure 16). The ions strike the dynode and release particles. An electron multiplier captures and amplifies these secondary particles producing the signal that the instrument associates with the ions that are responding to the mass-dependent instability.

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 12 500 u/s (for unit resolution). As the main RF voltage increases, ions of increasing mass-to-charge ratio become successively unstable in the axial 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 with the ion detection system detecting many of these ejected ions.

Voltages Applied to the Mass Analyzer End Caps

The ion isolation waveform, resonance excitation, and resonance ejection signals are AC voltages that are applied to the end caps (see Figure 16) to stimulate motion of the ions in the direction of the ion detection system. The voltages applied to the end caps are equal in amplitude but are 180° out of phase with each other. When the AC frequency applied to the end caps 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 (through the hole in one of the end caps as shown in Figure 16). The ion detection system consists of the conversion dynode and electron multiplier (Figure 15 and Figure 16).

The waveform signal needed for ion isolation consists of a distribution of frequencies between 5 and 425 kHz, containing all resonance frequencies except for those corresponding to the ions to be trapped. The ion isolation waveform acts during the ion isolation step of SIM, SRM, CRM, or MS^n (n > 1) full–scan applications. The waveform for ion isolation, 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 LCQ Fleet calculates and automatically applies the correct waveform voltage at the correct time.

During the collision–induced dissociation step of SRM, CRM, or MS^n (n > 1) full–scan applications, the resonance excitation signal is applied to the end caps to fragment parent ions into product ions. The signal 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 that 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 AC voltage for resonance ejection facilitates the ejection of ions from the mass analyzer and thus improves mass resolution. The AC 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 signal. 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 Gas in the Mass Analyzer Cavity

The mass analyzer cavity contains helium that is used as a damping gas and as a collision activation partner. The helium damping gas enters the mass analyzer cavity through a passage in the end cap. An open split regulates the flow of gas (approximately 1 mL/min) into the mass analyzer cavity, while the openings in the mass analyzer restrict the flow of gas out of the mass analyzer cavity (and into the turbomolecular pump). 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 the proper pressure.

As the ions enter the mass analyzer, they collide with the helium atoms and lose kinetic energy, which allows the RF field in the mass analyzer to trap them. As the ions continue to collide with the helium atoms, the amplitude of their oscillations decreases and they become focused towards the center of the trap, which significantly enhances sensitivity and mass spectral resolution.

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 AC voltage (used to induce resonance excitation) applied to the end caps 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.

Operation of the Mass Analyzer During Mass Analysis

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

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.

- Ion Storage

  Before ion storage, helium is present in the mass analyzer cavity, and the main RF voltage is set to the storage voltage. The ion isolation waveform voltage, resonance excitation AC voltage, and resonance ejection AC voltage on the end caps 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.

- Ion Isolation (SIM, SRM, CRM, or MS^n [n > 1] full scan only)

  Next, the ion isolation waveform voltage is applied to the end caps, 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.

- Collision induced dissociation (SRM, CRM, or MS^n [n > 1] full scan only)

  Then, for SRM, CRM, or MS^n (n > 1) full–scan analyses, the resonance excitation AC voltage is applied to the end caps 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.

- Ion scan out (the ion detection step)

  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 AC voltage is applied to the end caps to facilitate ejection. As the main RF voltage increases, 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 LCQ Fleet is equipped with one high sensitivity, on-axis ion detection system that produces a high signal-to-noise ratio and allows for voltage polarity switching between positive ion and negative ion modes of operation. The ion detection system includes a 15-kV conversion dynode and a channel electron multiplier. The ion detection system is located behind the mass analyzer (see Figure 15 and Figure 16).

Figure 17 shows the details of the ion detection system. 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. The curved surface of the conversion dynode focuses these secondary particles, and a voltage gradient accelerates them into the electron multiplier. The conversion dynode shield and disk shield the vacuum manifold from the electric field that the conversion dynode produces.

The electron multiplier is mounted on the top cover plate of the vacuum manifold behind the mass analyzer. See Figure 17 and Figure 21. 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

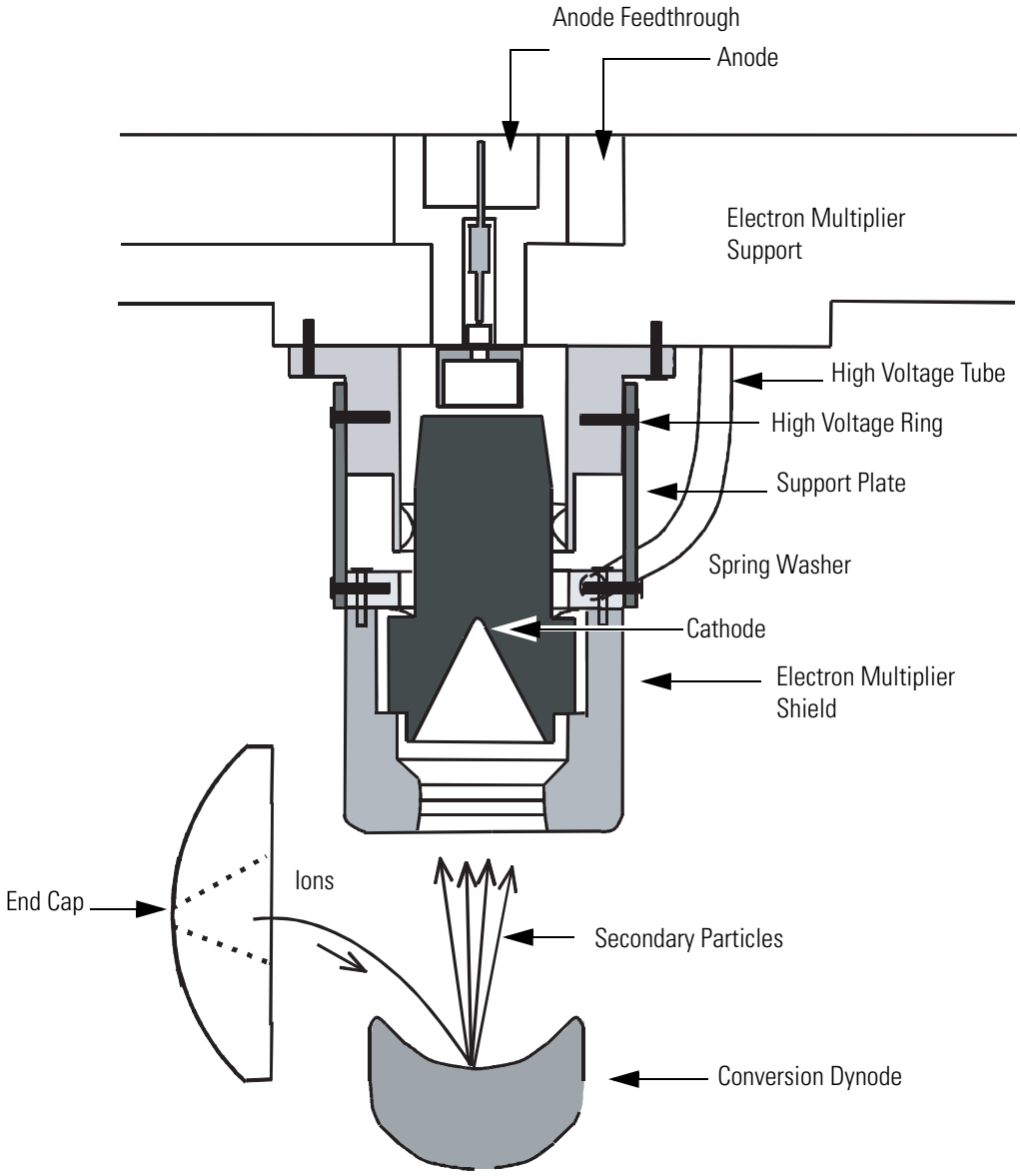
shield. A spring washer applies a force to the cathode to hold it in contact with the electron multiplier shield. Two screws attach the electron multiplier support to the top cover plate of the vacuum manifold.

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. The resulting cascade of electrons creates a measurable current at the end of the cathode where the anode collects the electrons. 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 4×10^5 (for example, for each ion or electron that enters, 4×10^5 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 "Ion Detection System Electronic Assemblies" on page 53.

Figure 17. Cross–sectional view of the ion detection system



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

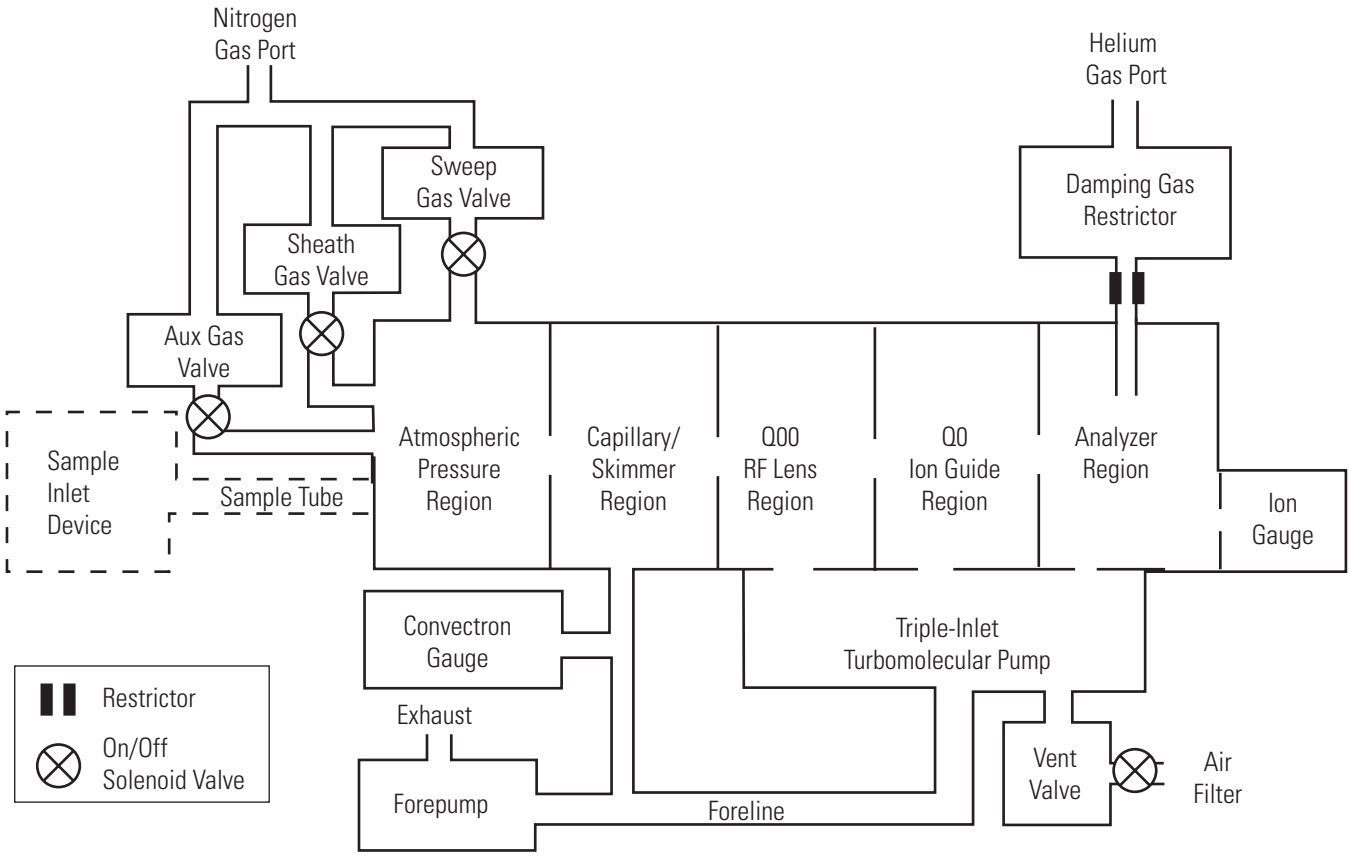
Vacuum System and API Source Gas Hardware

The vacuum system evacuates the region around the API stack, ion optics, mass analyzer, and ion detection system. The vacuum system and API source gas hardware includes the following components:

- Vacuum Manifold
- Turbomolecular Pump
- Forepump
- Convectron® Gauge
- Ion Gauge
- Vent Valve
- Damping Gas Inlet Assembly
- API Source Gas Hardware

Figure 18 shows a functional block diagram of the vacuum system and API source gas hardware.

Figure 18. Vacuum system and inlet gas hardware (functional block diagram)



Vacuum Manifold

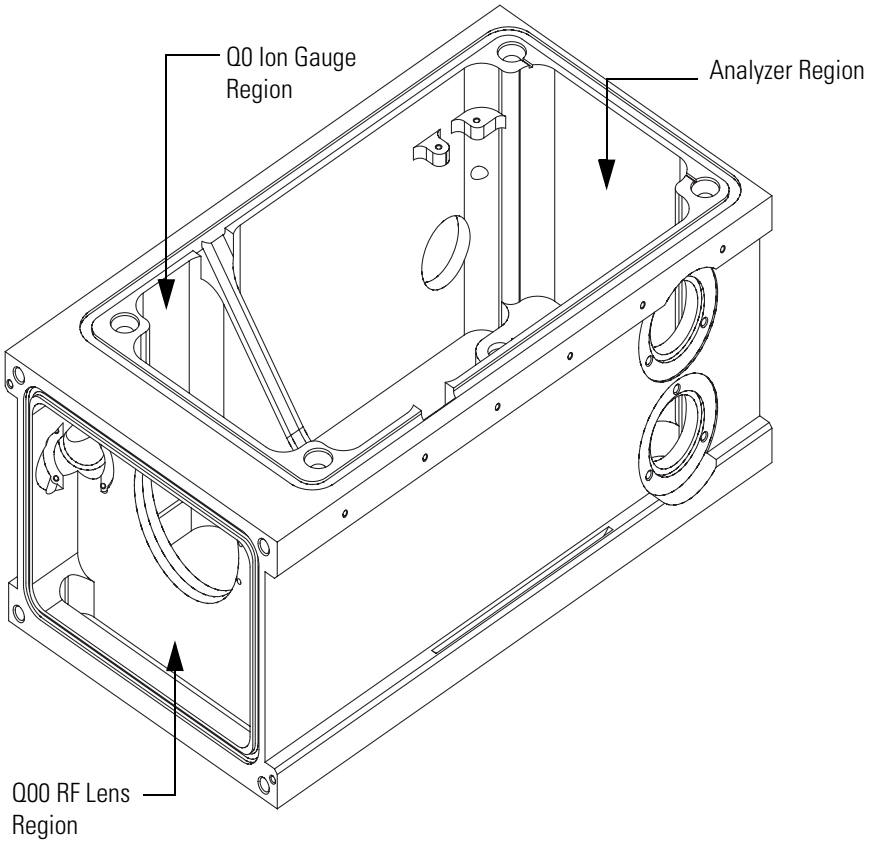
The vacuum manifold encloses the ion source interface, ion guides, mass analyzer, and ion detection system assemblies. The vacuum manifold is a thick-walled, aluminum chamber with a removable top cover plate, machined flanges on the front, sides, and bottom, and various electrical feedthroughs and gas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

The vacuum manifold is divided into four chambers by three baffles. Figure 19 shows three of these chambers. The forepump evacuates the capillary/skimmer region inside the first chamber. The third inlet in the molecular drag section of the triple-inlet turbomolecular vacuum pump evacuates the Q00 RF lens region. The interstage port of the turbomolecular vacuum pump evacuates the Q0 ion guide region. The high vacuum port of the turbomolecular pump evacuates the analyzer region. In turn, the turbomolecular pump discharges into the forepump through the foreline.

Three high-voltage electrical feedthroughs pass through the vacuum manifold, one feed-through for each of the following:

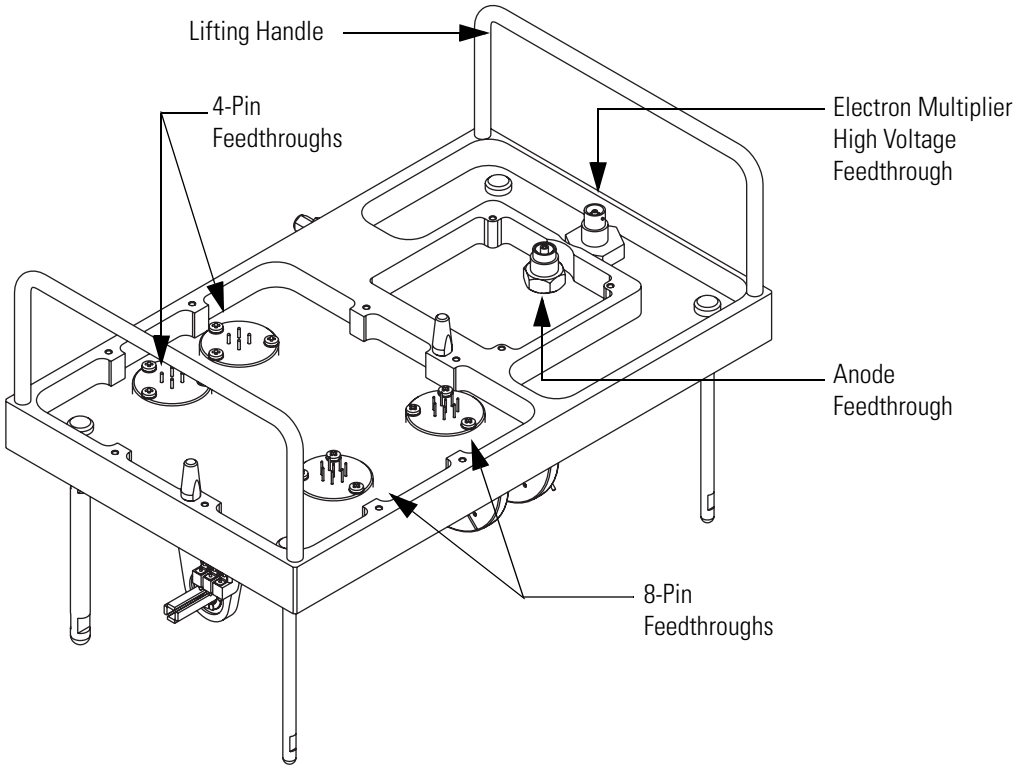
- The conversion dynode high voltage
- The RF voltage of the mass analyzer
- The AC voltages of the mass analyzer

Figure 19. Vacuum manifold



The removable top cover plate of the vacuum manifold holds the Q0 and Q1 ion guides, the electron multiplier (part of the ion detection system), and ion trap. Removing of the top cover plate gives you access to these assemblies. The top cover plate has two handles on the top and four guide posts on the underside to facilitate its removal and installation. An O-ring provides a vacuum-tight seal between the top cover plate and the vacuum manifold. Figure 20 and Figure 21 show the top cover plate and its attached assemblies.

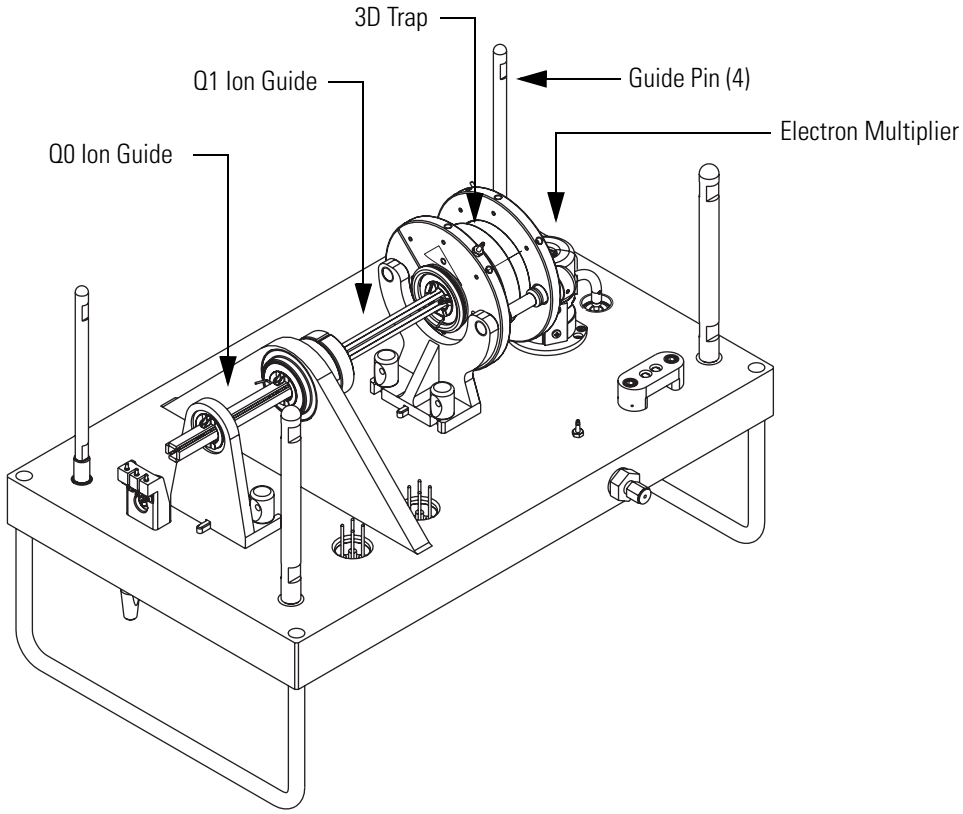
Figure 20. Top cover plate of the vacuum manifold (topside)



Six electrical feedthroughs pass through the top cover plate:

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

Figure 21. Top cover plate of the vacuum manifold (underside), and attached assemblies



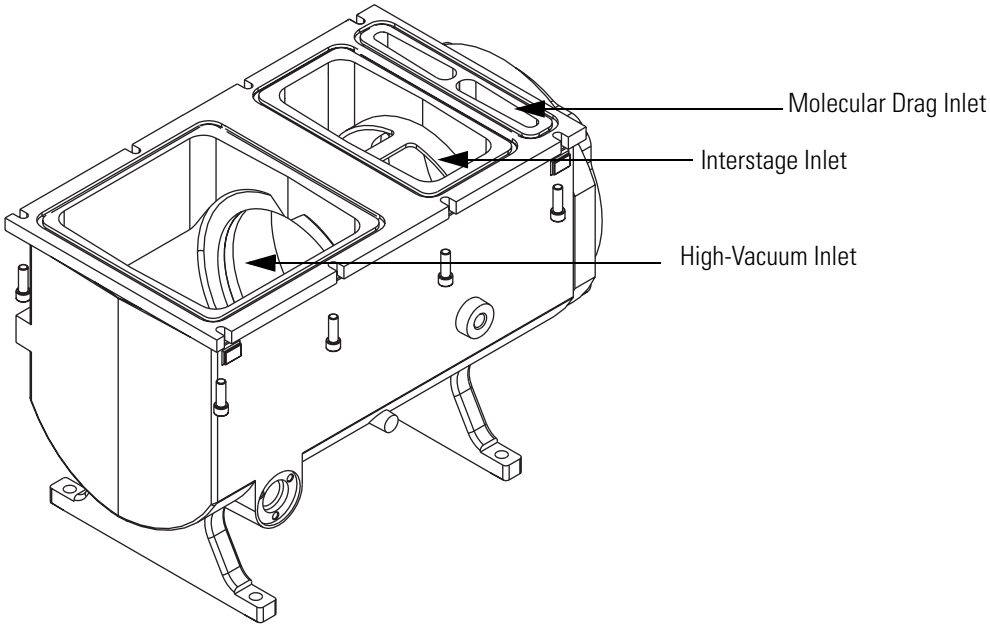
Turbomolecular Pump

A Leybold TW220/150/15S triple-inlet turbomolecular pump provides the vacuum for the Q00 RF lens 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 22):

- A 220 L/s high-vacuum inlet at the top of the rotor stack, which evacuates the analyzer chamber
- A 150 L/s interstage inlet about half way down the rotor stack, which evacuates the Q0 ion guide chamber
- A 15 L/s third inlet in the molecular drag section of the pump, which evacuates the Q00 RF lens chamber

Figure 22. Turbomolecular pump



The turbomolecular pump is controlled by a Leybold TDS controller and powered by a +24 V dc power supply. The main power circuit breaker switch turns off the power for the turbomolecular pump, not the electronics service switch. A fan that draws air in from the front of the instrument cools the pump.

The Leybold TDS Turbomolecular Pump Controller provides power to and control of the turbomolecular pump. The turbomolecular pump status (such as the temperature or rotational speed) 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 pump temperature is too high.

Forepump

An Edwards E2M30 forepump (also referred to as a rotary-vane pump or a 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 1 Torr.

A section of 1.27 cm (0.5 in.) ID reinforced PVC tubing connects the forepump to the turbomolecular pump. The power cord of the forepump is plugged into the outlet labeled Mech. Pumps on the power panel (see Figure 11 on page 28). 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.

Ion Gauge

A Granville-Phillips® 342™ mini ion gauge measures the pressure in the analyzer region of the vacuum manifold. 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 used 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. A power failure or placing the main power circuit breaker in the Off (O) position removes power from the MS detector. After the external power is removed, power is provided to the vent valve for a short time. If external power is not restored to the MS detector in 10 seconds, however, power to the vent valve solenoid shuts off. When power to the vent valve solenoid shuts, the vent valve opens and the manifold is vented to filtered air. The vent valve closes after power to the MS detector is restored.

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 back of the MS detector. The LCQ Fleet regulates the flow of helium by use of an open split helium line. The helium enters the mass analyzer through a nipple on the ion trap mount.

Helium in the mass analyzer cavity dampens ionic motion and improves the performance of the MS detector. See "Helium Gas in the Mass Analyzer Cavity" on page 37.

API Source Gas Hardware

The source gas hardware controls the flow of sheath gas, auxiliary gas, and sweep gas into the MS detector.

The sheath gas, auxiliary gas, and sweep gas valves control the flow of nitrogen into the API source. Sheath gas is nitrogen gas that flows through the inner coaxial of the API probe. The sheath gas converts the sample solution into a fine mist as the solution exits the sample tube. Auxiliary gas is the outer coaxial nitrogen gas that assists the sheath gas in the evaporation of the sample solution. Sweep gas flows out from behind the sweep cone in the ion source interface. The 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 back of the MS detector. Valves that are controlled by the data system regulate the nitrogen pressure. You can set the flow rates from the Tune Plus window. Sheath gas is not used with an NSI source. The sheath gas, auxiliary gas, and sweep gas enter the API source through 1/4-in. ID tubing.

Cooling Fans

Five fans provide cooling for the MS detector: a 100 $ft.^3$/min fan cools the RF voltage coil; a 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 back 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, always operate the MS detector 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. These other modules are 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 Entry Module and Power Distribution
- 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 11 on page 28.

The Power Entry Module accepts, filters, and provides line power to various components of the MS detector. Figure 23 shows a functional block diagram of the Power Entry Module and MS detector power distribution.

The Power Entry Module includes the following components:

- **Main power circuit breaker switch**. 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, and passes through the main power circuit breaker and a line filter (see Figure 11 on page 28). The main power circuit breaker switch, located on the right side panel of the MS detector (see Figure 11 on page 28), 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.
- **Line filter**. The line filter removes noise from the line power.
- **Electronics service switch**. 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 while the vacuum system is still in operation (see Figure 11 on page 28). 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, all components of the MS detector receive power.
- **Interlock PCB**. The interlock PCB, which resides in the Power Entry Module, receives 220 V ac from the electronics service switch (called service 220 V ac) and +24 V dc from PS2 power supply by way of 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 8 KV power supply and the power supply of the conversion dynode and electron multiplier.

CAUTION 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 power/signal distribution PCB receives 220 V ac and service 220 V ac from the Power Entry 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, the turbomolecular pump, the 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 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.

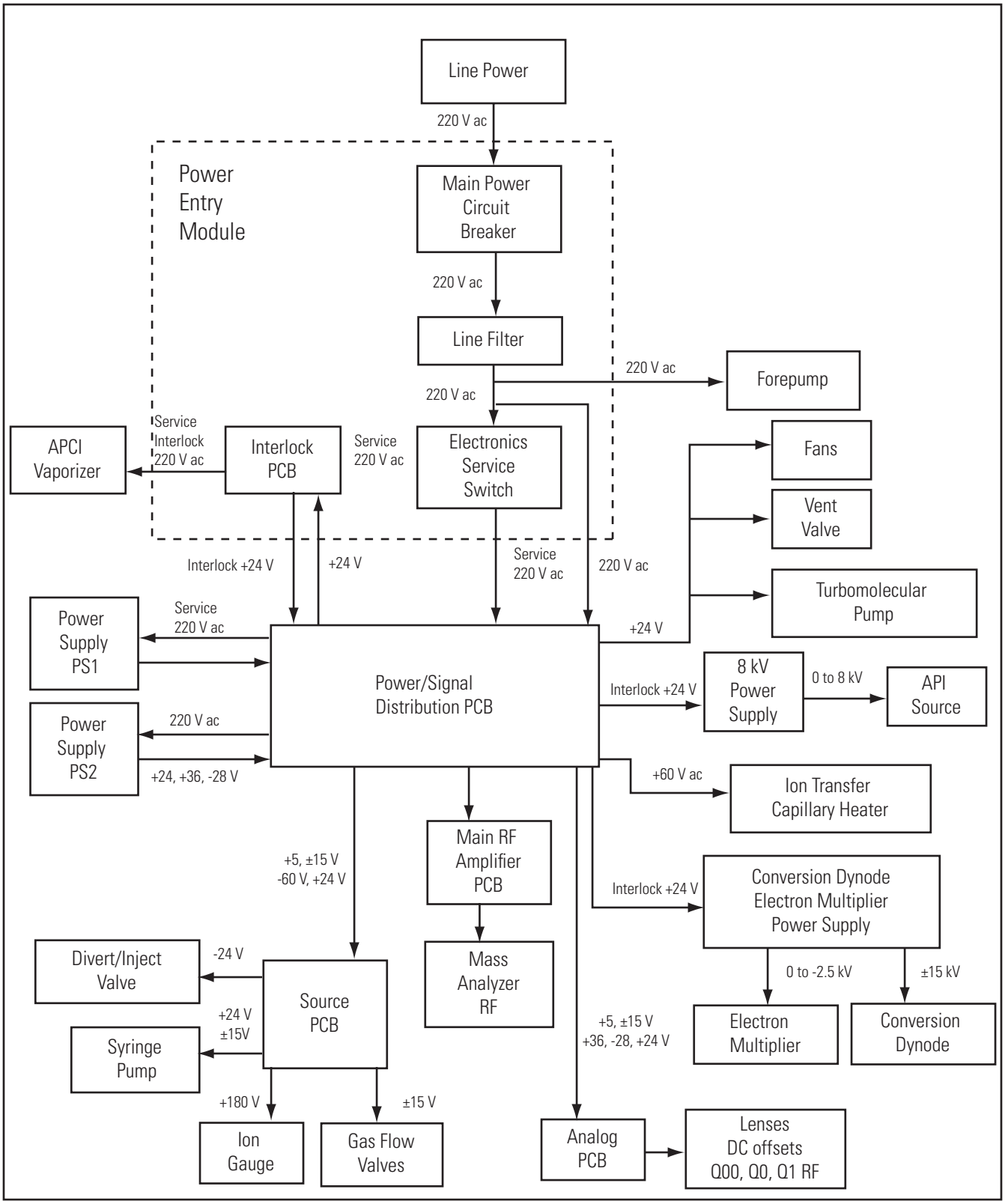
Power supply PS2 provides +24 V dc for the turbomolecular pump, fans, vent valve, divert/inject valve, syringe pump, 8 KV power supply, conversion dynode/electron multiplier power supply, main RF PCB, and analog PCB. It also provides +36 V dc and -28 V dc that are used for RF generation for the ion guides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

The source PCB distributes power to the ion gauge, divert/inject valve, syringe pump, and nitrogen 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 dynode and 0 to –2.5 KV to the electron multiplier in the ion detection system.

Figure 23. Functional block diagram of the Power entry module and power distribution of the MS detector



System Control and Monitoring Circuitry

Table 2 lists the LCQ Fleet electronic circuitry that controls and monitors the operation of the MS detector.

Table 2. System control and monitoring circuitry, (Sheet 1 of 2)

Circuit	Function
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.
Divert/inject valve control circuit	Controls and monitors the divert/inject valve.
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.
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.
Conversion dynode control circuit	Controls and monitors the polarity of the 15 kV potential that is applied to the conversion dynode.
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.
APCI vaporizer heater/sensor control circuit/safety interlock relay	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.
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.
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.
RF voltage control circuitry	Controls and monitors the PCBs that are responsible for RF voltage generation.
Temperature monitoring circuitry	Monitors the temperatures at several PCBs in the MS detector.
Diagnostic circuitry	Monitors the outputs of various components and circuits on the LCQ Fleet. Information on voltages, currents, temperatures, flow rates, logic, and so on is sent to the data system, where it can be accessed in the diagnostics views of Tune Plus.

Table 2. System control and monitoring circuitry, (Sheet 2 of 2)

Circuit	Function
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 any of these components: 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, or shuts down dc voltages to the ion transfer capillary heater, tube lens, ion optics, and mass analyzer, if one or more of the following conditions occurs: • 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 API probe has been removed). The Vacuum LED on the LCQ Fleet front panel is illuminated green when the vacuum protection circuitry detects adequate vacuum.

RF / Waveform Voltage Generation Electronic Assemblies

The RF/waveform voltage generation electronic assemblies produce the RF voltages for the mass analyzer, Q00 RF lens and Q0 quadrupole, 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 end caps of the mass analyzer.

The main RF voltage generation involves the following components:

- **RF oscillator located on the digital PCB**. This oscillator provides a 825 kHz sine wave reference signal that it uses to produce the RF voltage.
- **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.
- **Low pass filter PCB**. Removes second and third harmonics from the RF primary voltage.
- **RF voltage coil.** Amplifies the RF primary voltage to produce a secondary voltage of 0 to 10 000 V ac (zero to peak) that is supplied to the rods of the mass analyzer.
- **RF voltage detector**. Senses the 0 to 10 000 V RF voltage signal that is applied to the rods of the mass analyzer and converts this sensed signal into a 0 to -10 V dc output signal.

- **Mass DAC and Integrating amplifier**. This 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.
- **Waveform AWG (arbitrary waveform generator)**. Part of the digital PCB, the waveform AWG provides the reference waveforms that are used to create the ion isolation waveform voltage, resonance excitation RF voltage, and resonance ejection RF voltage. A waveform amplifier on the analog PCB amplifies the reference waveforms. The embedded computer, 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 electron multiplier and conversion dynode of the ion detection system. The ion detection system electronic assemblies also receive the electron multiplier output current signal, convert it to a voltage (by the electrometer circuit), and pass it to the data system. Figure 24 shows a functional block diagram of the ion detection system electronic assemblies.

The ion detection system electronic assemblies include the following:

- Electron multiplier/conversion dynode power supply

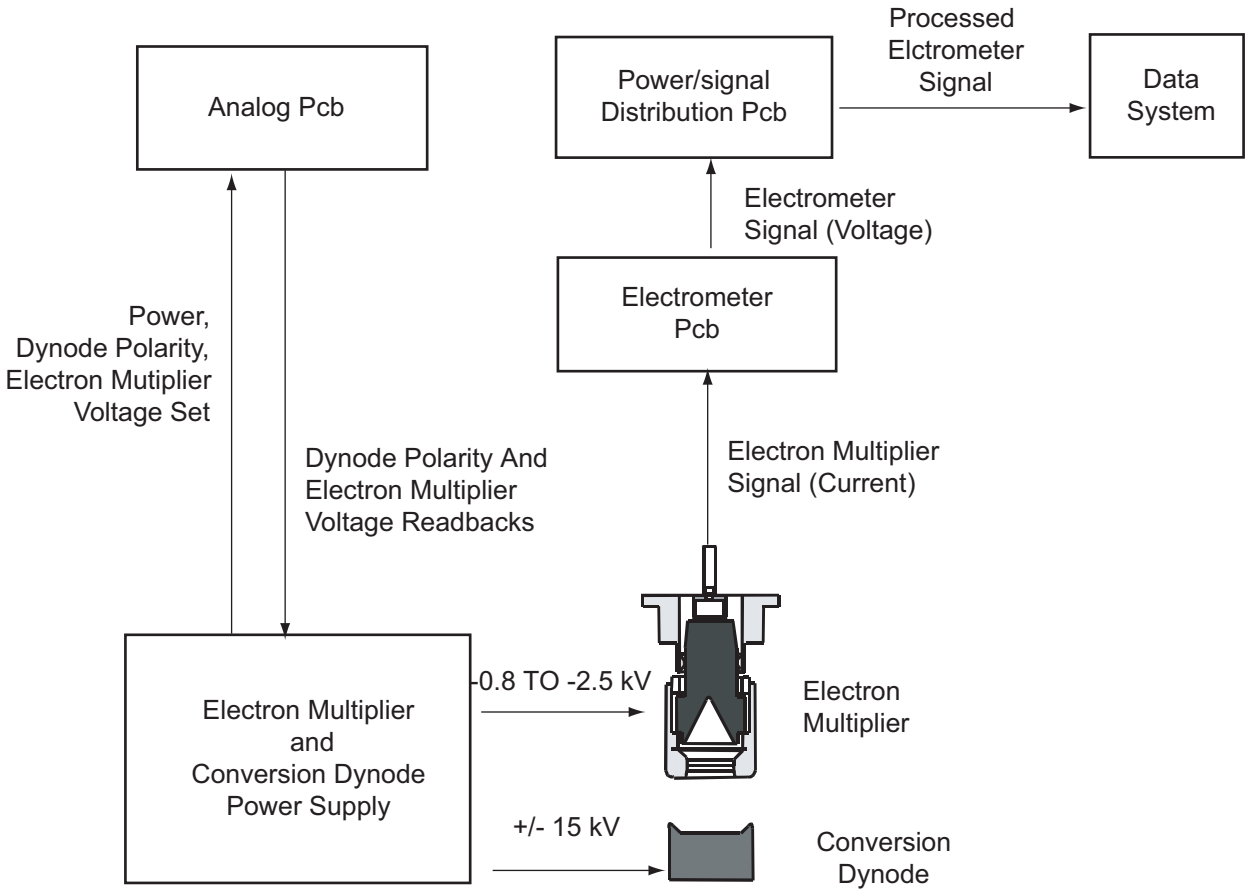
  The electron multiplier/conversion dynode power supply supplies the -0.8 kV to -2.5 kV dc high voltage to the cathode of the electron multiplier. The high voltage set control signal for the electron multiplier power supply comes from the analog PCB. This signal controls a feedback control circuit and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

  The electron multiplier/conversion dynode power supply also supplies +15 kV and -15 kV dc high voltage to the conversion dynode. A control signal from the analog PCB determines the polarity of the voltage applied to the conversion dynode.

- Electrometer circuit

  The electrometer circuit, located in a shielded enclosure on the electrometer PCB, receives the amplified ion current from the anode of the electron multiplier, converts the current into a voltage, and then integrates the voltage over time. The integrated voltage is then passed to the power/signal distribution PCB where it is processed and sent to the data system.

Figure 24. Ion detection system electronic assemblies (functional block diagram)



Data System

The data system controls and monitors the LCQ Fleet. The data system also processes data that the LCQ Fleet acquires.

This section contains the following topics:

- Software and Computer Hardware Requirements
- Data System/ MS Detector and Local Area Network Interface
- Printer

Software and Computer Hardware Requirements

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

Table 3 lists the minimum software and computer hardware requirements to install the LCQ Fleet 2.4 instrument control software and the Xcalibur 2.0.5 data system.

Table 3. Software and computer hardware requirements for running Xcalibur 2.0.5 and higher

Computer hardware	Software
Intel Pentium IV 1 GHz processor	Microsoft Windows XP SP2
256 MB RAM for processing	Microsoft Office XP 2003
256 MB RAM for acquisition	
20 GB hard drive (NTFS) or more recommended	
CD-ROM drive	
Video card and monitor capable of 1280 × 1025 resolution and 65 536 colors	

Data System/ MS Detector and Local Area Network Interface

The data system computer contains two Ethernet adapters; one adapter is labeled User's Network and the other adapter is labeled Surveyor MS.

Use the Ethernet adapter that is labeled User's Network to connect to your local area network.

Use the Ethernet adapter that is labeled Surveyor MS to connect to a a 10/100 base T Ethernet switch. Connect the LCQ Fleet MS detector, Surveyor Autosampler, Surveyor LC Pump Plus, and Surveyor PDA Plus Detector to the Ethernet switch.

Note The Surveyor MS Pump Plus communicates with the data system computer through a USB connection.

Printer

A high-resolution laser printer is available with the LCQ Fleet as an option. The printer communicates with the PC via the local area network. Refer to the printer manual for details.

❖ To set up the printer

Choose **File > Print Setup** from any window in the Xcalibur data system or the Tune Plus program.

The Print Setup dialog box appears.

Daily Operation

To ensure the proper operation of your system, Thermo Scientific recommends that you perform daily preventative maintenance. This chapter provides details about the items you should check before you operate the system and the cleaning procedures you should perform after you complete your analyses and contains the following sections:

- Before Operating the LCQ Fleet
- After Operating the LCQ Fleet

Note You do not need to tune (optimize the tune parameters for the ESI calibration solution) and calibrate the LCQ Fleet 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 must tune and calibrate the LCQ Fleet (that is, optimize the tune for the ESI calibration solution and calibrate the mass accuracy using the ESI calibration solution) about once a quarter.

You must optimize the tune parameters (create a new tune method) whenever you change the type of experiment.

For information on tuning and calibration, refer to the *LCQ Fleet Getting Started Guide*.

Before Operating the LCQ Fleet

Perform the following procedures every day before you begin your first analysis:

- Checking the Helium and Nitrogen Supplies
- Checking the ESI Fused-Silica Sample Tube for Elongation
- Checking the System Vacuum Levels
- Checking the Disk Space

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.

CAUTION Before you begin normal operation each day, make sure 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. The LCQ Fleet displays a popup message when the nitrogen pressure is too low.

Checking the ESI Fused-Silica Sample Tube for Elongation

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

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

❖ To cut and reposition the end of the sample tube

1. Remove the ESI probe from the Ion Max-S ion source.

   For instructions on removing the ESI probe, refer to the *Ion Max and Ion Max-S 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. With a fused-silica cutting tool, 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 recessed just inside the ESI needle by approximately 1 mm. If necessary, loosen the fitting and reposition the sample tube.

8. Reinstall the ESI probe.

   For instructions on installing the ESI probe, refer to the *Ion Max and Ion Max-S API Source Hardware Manual*.

Checking the System Vacuum Levels

For proper performance, you must operate the LCQ Fleet system 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. Before you begin daily operation, check for major air leaks in the system, and check the vacuum levels of the system.

❖ To check the system for major air leaks

Listen for a rush of air or a hissing sound inside the MS detector.

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.

❖ To check the system vacuum levels

1. From the Windows XP taskbar, choose **Start > All Programs > Xcalibur > LCQ Fleet Tune**.

   The Tune Plus window appears.

2. Choose **Setup > Vacuum**.

   The Vacuum dialog box appears.

3. Check the Convectron Gauge Pressure readback. This readback displays the current pressure in the capillary-skimmer and foreline region.

4. Check the Ion Gauge Pressure readback. This readback displays the current pressure in the analyzer region.

5. Compare the current values of the pressures in the vacuum manifold with the values listed in Table 4.

   If the observed pressures are higher than those in the table, your system might have an air leak. 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 decreases with time, check the pressure periodically until it falls within the typical pressure range of the MS detector. If the pressure remains high, your system might have an air leak.

Table 4. 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

❖ **To remedy an air leak**

1. Shut down the system as described in Shutting Down the System Completely on page 113.
2. Make a visual inspection of the vacuum system and vacuum lines for leaks.
3. Check each fitting and flange on the system for tightness, and tighten the fittings or flanges that are loose. Do not tighten fittings indiscriminately. Pay particular attention to fittings that have been changed recently or to fittings that have been subjected to heating and cooling.
4. Make sure that the cover plates of the vacuum manifold are properly seated.

Checking the Disk Space

Periodically verify that your hard disk drive has enough free space for data acquisition.

❖ **To determine the amount of available disk space**

1. From the Windows XP Start menu, choose **All Programs > Xcalibur > Xcalibur**.

   The Xcalibur Home Page window appears.
2. Choose **Actions > Check Disk Space**.

   The Disk Space dialog box appears and lists the following:

   - Current drive and directory (for example, C:\Xcalibur\system\programs)
   - Number of Mb that are available (free) on the current drive
   - Percentage of the current drive that is available
   - Total capacity of the current drive
3. To select another disk drive so that you can determine its disk space, click **Directory**.

4. When you have completed this procedure, click **OK** to close the dialog box.

Tip 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.

After Operating the LCQ Fleet

After operating the LCQ Fleet, perform the following procedures in sequence:

1. Flushing the Sample Transfer Line, Sample Tube, and API Probe
2. Placing the System in Standby Mode
3. Flushing the Ion Sweep Cone and Ion Transfer Capillary
4. Purging the Oil in the Forepump
5. Emptying the Solvent Waste Bottle

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

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) with a mobile phase of 50:50 methanol \ distilled water. Flushing the system with 50:50 methanol \ distilled water at at a flow rate of 200 to 400 µL/min for a period of approximately 15 minutes should be sufficient to remove contamination.

❖ **To flush the sample transfer line, sample tube, and API probe**

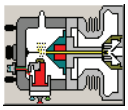
1. Wait until data acquisition, if any, is complete.
2. Make sure that the lid to the API chamber is closed and secured.
3. From the Windows XP taskbar, choose **Start > All Programs > Xcalibur > LCQ Fleet Tune**.

   The LCQ Fleet Tune Plus window appears.



On Standby

4. From the Tune Plus window, choose **Control > On** (or click 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. To set up the APCI source to be flushed



   a. In the LCQ Fleet Tune Plus window, choose **Setup > APCI Source** (or click the APCI Source button).

The APCI Source dialog box appears.

b. To set the APCI vaporizer temperature to 500 °C, type **500** in the Vaporizer Temperature box.

c. To set the sheath gas flow rate to 30, type **30** in the Sheath Gas Flow Rate box.

d. To set the auxiliary gas flow rate to 5, type **5** in the Aux Gas Flow Rate box.

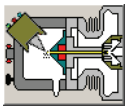
e. To set the sweep gas flow rate to 0, type **0** in the Sweep Gas Flow Rate box.

f. To set the APCI spray current to 0, type **0** in the Spray Current box.

g. Click **OK**.

h. Go to step 7.

6. To set up the ESI source to be flushed



a. In the LCQ Fleet Tune Plus window, choose **Setup > ESI Source** (or click the ESI source button).

The ESI Source dialog box appears.

b. To set the sheath gas flow rate to 30, type **30** in the Sheath Gas Flow Rate box.

c. To set the auxiliary gas flow rate to 5, type **5** in the Aux Gas Flow Rate box.

d. To set the sweep gas flow rate to 0, type **0** in the Sweep Gas Flow Rate box.

e. To set the ESI spray voltage to 0, type **0** in the Spray Voltage box.

f. Click **OK**.

7. To set up and start a flow of 50:50 methanol \ water solution from the LC to the API source:

a. In the LCQ Fleet Tune Plus window, choose **Setup > Inlet Direct Control** (or click **AS/LC direct control**).

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 50% water.

e. Click  (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 minutes.

9. After 15 minutes, turn off the flow of liquid from the LC to the API source as follows:

a. Leave the API source (including the APCI vaporizer, sheath gas, and auxiliary gas) on for an additional 5 minutes.

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

10. After 5 minutes, turn off the API source by placing the MS detector in Standby. From the LCQ Fleet Tune Plus window, choose **Control > Standby** (or click **On/Standby**) to put the MS detector in Standby.

Placing the System in Standby Mode

❖ **To place the LCQ Fleet system in Standby mode**

1. From the LCQ Fleet Tune Plus window, choose **Control > Standby** (or click **On/Standby**) to put the MS detector in Standby.

   The System LED on the front panel of the MS detector turns yellow when the system is in Standby.

2. Leave the MS detector power On.
3. Leave the LC pump power On.
4. Leave the autosampler power On.
5. Leave the data system power On.

Flushing the Ion Sweep Cone and Ion Transfer Capillary

You must 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 pump a solution of 50:50 methanol \ water solution through the sample transfer line, sample tube, and API probe (see Flushing the Sample Transfer Line, Sample Tube, and API Probe on page 61.) If you use a mobile phase that contains a nonvolatile buffer or inject high concentrations of sample, you might need to clean the ion sweep cone and ion transfer capillary more often. It is not necessary 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**

1. To turn off the solvent flow from the LC pump (or other sample introduction device) to the API source

   a. From the Windows XP taskbar, choose **Start > All Programs > Xcalibur > LCQ Fleet Tune**.

      The LCQ Fleet Tune Plus window appears.

   b. Choose **Setup > Inlet Direct Control** (or click **AS/LC direct control**).

      The Inlet Direct Control view appears.

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

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

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 approximately 20 minutes for the vaporizer and ion transfer capillary to cool to room temperature before you touch or remove either component.

3. Remove the Ion Max ion source from the front of the MS detector, as described in "Removing the Ion Max Ion Source Housing" on page 77.

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 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.

7. To remove the ion sweep cone (if it is installed)

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

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

Tip This is a good point to remove and clean the ion transfer capillary. You remove the ion transfer capillary by turning it counter clockwise with the custom removal tool. See Cleaning the Ion Transfer Capillary and Ion Sweep Cone on page 73.

8. To clean the ion transfer capillary and the ion sweep cone (if it is installed)

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

   b. Place the beaker in an ultrasonic bath, and sonicate these components for 15 minutes.

   c. Dry the ion sweep cone.

9. Clean the spray cone with a Kimwipe™ tissue soaked in methanol.

10. To reinstall the ion sweep cone
    a. Carefully align the gas inlet (see Figure 26) on the ion sweep cone with the sweep gas supply port (see Figure 25) in the API cone seal. Firmly press the ion sweep cone into position.
    b. If necessary, adjust the set screws around the perimeter of the ion sweep cone.

Figure 25. View of the sweep gas supply port in the API cone seal

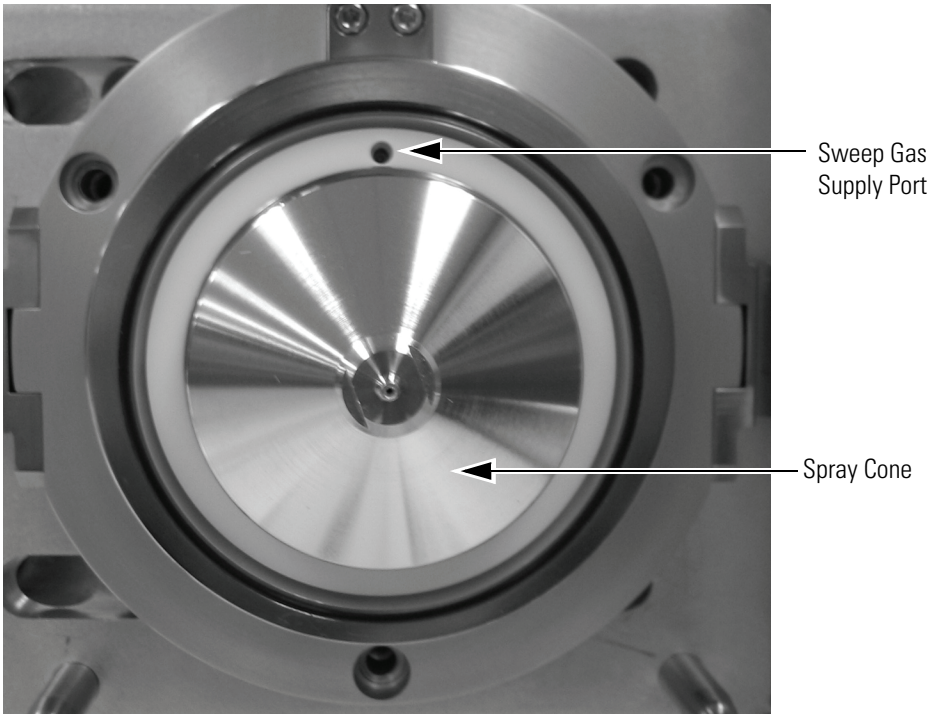
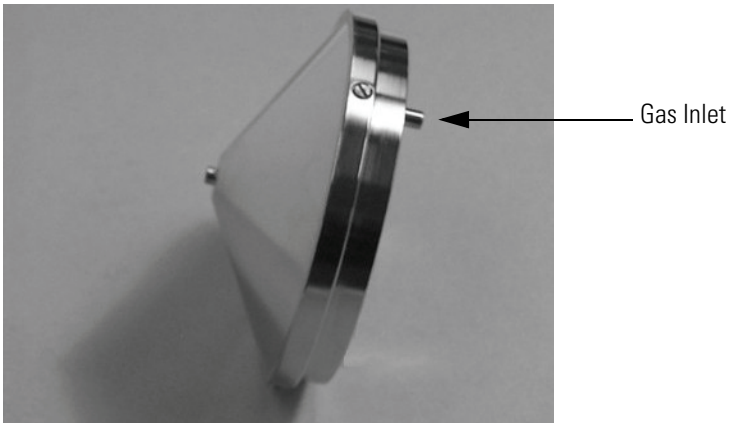


Figure 26. View of the gas inlet on the ion sweep cone



11. Reinstall the Ion Max ion source as described in "Reinstalling the Ion Max Ion Source Housing" on page 85.

Purging the Oil in the Forepump

Plan to purge (decontaminate) the oil in the forepump (also known as a rotary-vane pump, backing pump, roughing pump, or mechanical pump) on a daily basis to remove water and other dissolved chemicals from the pump oil. Water and other chemicals in the forepump can cause corrosion and decrease the lifetime of the forepump. The best 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 forepump

1. To turn off the solvent flow from the LC pump to the API source:
   a. From the Windows XP taskbar, choose **Start > All Programs > Xcalibur > LCQ Fleet Tune**.

      The LCQ Fleet Tune Plus window appears.
   b. Choose **Setup > Inlet Direct Control** (or click on the AS/LC direct control button).

      The Inlet Direct Control view appears.
   c. Click the LC tab and click  (or **Pump Off** or **Stop Pump**) to stop the LC pump.


On


Standby

2. From the LCQ Fleet Tune Plus window, choose **Control > Standby** (or click the **On/Standby** button) to put the MS detector in Standby.
3. Ensure that a septum seals the entrance to the ion transfer capillary.
4. Open the gas ballast valve on the forepump by turning it to position |.

   Refer to the manual that came with the forepump for the location of the gas ballast valve.
5. Allow the pump to run for 30 minutes with the gas ballast valve open.
6. After 30 minutes, close the gas ballast valve by turning it to position O.

Emptying the Solvent Waste Bottle

Check the solvent level in the solvent waste bottle on a daily basis. If necessary, empty the solvent waste bottle. Dispose of the solvent waste in accordance with local and national regulations.

MS Detector Maintenance

The performance of the LCQ Fleet MS detector depends on the maintenance of all parts of the instrument.

Note Table 5 and Table 6 list the maintenance procedures that you must perform on a regular basis to maintain your LCQ Fleet system. Table 7 lists the maintenance procedures that should be performed by a Thermo Scientific service engineer.

This chapter describes routine MS detector maintenance procedures that you or your Thermo Scientific service engineer must perform to ensure optimum performance of the instrument. Most of the procedures involve cleaning. Maintenance procedures include cleaning the API source, ion guides, mass analyzer, and ion detection system. Procedures are also provided for replacing the API sample tube, ion transfer capillary, and API source, ion optics, and mass analyzer assemblies.

This chapter contains the following sections:

Overview of Maintenance Procedures

To maintain the performance of the MS detector, you must perform the maintenance procedures listed in Table 5. When you perform these procedures, do the following:

- 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.

Table 5. User–performed MS detector maintenance procedures

MS Detector Component	Task	Frequency	Procedure
API source	Flush (clean) the sample transfer line, sample tube, and API probe	Daily	Flushing the Sample Transfer Line, Sample Tube, and API Probe on page 72
Ion source interface	Flush (clean) the ion sweep cone and ion transfer capillary	Daily (or more often[1])	Flushing the Ion Sweep Cone and Ion Transfer Capillary on page 72
	Clean the tube lens and skimmer	As needed[1]	Cleaning the Tube Lens and Skimmer on page 79
	Remove and clean the ion transfer capillary	Weekly, or if the ion transfer capillary bore is contaminated or blocked	Cleaning the Ion Transfer Capillary and Ion Sweep Cone on page 73
	Replace the ion transfer capillary	If its bore is corroded	*Ion Max and Ion Max-S API Source Hardware Manual*
PhotoMate light source	Clean or polish the VUV lamp window	If the VUV lamp window is dirty	*Ion Max API Source Hardware Manual*
	Replace the VUV lamp	If the lamp fails	*Ion Max and Ion Max-S API Source Hardware Manual*
Cooling fans	Clean the fan filters	Every 4 months	Cleaning the Fan Filter on page 110
ESI probe	Trim the sample tube	If polyimide coating on the end of the sample tube has elongated	Checking the ESI Fused-Silica Sample Tube for Elongation on page 58
APCI or ESI probe	Replace the sample tube	If sample tube is broken or obstructed	*Ion Max and Ion Max-S API Source Hardware Manual*
Ion detection system	Clean the ion detection system (electron multiplier and conversion dynode)	Whenever you remove the top cover plate of the vacuum manifold	Cleaning the Ion Detection System on page 99

[1]Frequency depends on analytical conditions

To keep the forepump (also known as a rotary-vane pump or mechanical pump) in optimal working condition, you must perform the maintenance procedures listed in Table 6.

Table 6. User performed forepump maintenance procedures

Task	Frequency	Procedure
Purge (decontaminate) oil	Daily	Purging the Oil in the Forepump on page 66
Add oil	When the oil level is low	Manufacturer's documentation
Change oil	Every 3 months, or if oil is cloudy or discolored	Manufacturer's documentation

Because the procedures listed in Table 7 require a system shutdown and the removal of one or more of the outer covers of the MS detector, they must be performed by aThermo Scientific service engineer.

Table 7. MS detector maintenance procedures that should be performed by a Thermo Scientific Service Engineer

MS Detector Component	Procedure	Frequency	Procedure
Ion detection system	Replace the electron multiplier assembly	If noise in spectrum is excessive or proper electron multiplier gain can not be achieved	Replacing the Electron Multiplier on page 105
Q0 ion guide	Clean Q0 quadrupole and intermultiple lens L1	As needed[1]	Cleaning the Q0 and Q1 Ion Guides on page 91
Mass analyzer	Clean the mass analyzer	Rarely (if ever)[1]	Maintaining the Mass Analyzer on page 101
Q1 ion guide	Clean the Q1 octapole and gate lens	As needed[1]	Cleaning the Q0 and Q1 Ion Guides on page 91
Q00 RF lens	Clean Q00 RF lens and lens L0	As needed[1]	Maintaining the Internal Components of the Ion Source Interface on page 76
Turbomolecular pump	Replace the turbomolecular pump insert	Every 20 000 to 30 000 hours or if bearings fail	Replacing the Turbomolecular Pump Cartridge on page 109
PCBs	Replace PCB	If PCB fails	
Electronic modules	Replace the module	If the electronic module fails	

Tools and Supplies

The LCQ Fleet requires very few tools to perform routine maintenance. You can remove and disassemble many of the components by hand. The tools, equipment, and chemicals listed in Table 8 are needed for the maintenance of the API source, ion guides, mass analyzer, and ion detection system.

Table 8. Tools, equipment, and chemicals required for maintenance

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 Make sure that solvents and reagents are stored and handled according to standard safety procedures and disposed of according to applicable local and national regulations.

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 an MS detector component is to the source of the ions, the more rapidly it becomes dirty. Table 9 lists the frequency of cleaning for the component of the MS detector.

Table 9. Frequency of cleaning for the components of the MS detector

Component	Frequency of cleaning	Procedure
Sample tube, API probe, ion transfer capillary bore, ion sweep cone of the API source	Clean 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.	Flushing the Sample Transfer Line, Sample Tube, and API Probe on page 72 Flushing the Ion Sweep Cone and Ion Transfer Capillary on page 72
Tube lens and skimmer of the Q00 RF lens and lens L0	Clean occasionally.	Cleaning the Q00-L0 RF Lens on page 87
Q0 quadrupole, Q1 octapole, and lenses of the Q0 and Q1 ion guides	Clean occasionally.	Cleaning the Q0 and Q1 Ion Guides on page 91
Electrodes of the mass analyzer	Clean rarely.	Maintaining the Mass Analyzer on page 101
Electron multiplier and conversion dynode	Whenever you remove the top cover plate of the vacuum manifold, clean these components by blowing them with a clean, dry gas.	Cleaning the Ion Detection System on page 99

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

1. The API probe, ion sweep cone (if installed), spray cone, and ion transfer capillary
2. The tube lens and skimmer
3. The quadrupole and lens of the Q00 RF lens
4. The quadrupole and lens of the Q0 ion guide and the octapole and lens of the Q1 ion guide
5. The mass analyzer

API Source Maintenance

The API source requires minimal maintenance. Periodically, you must 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.

For information on maintaining the API probes or the Photomate light source, refer to the *Ion Max and Ion Max-S API Source Hardware Manual*.

This section contains maintenance procedures for the following:

- Flushing the Sample Transfer Line, Sample Tube, and API Probe
- Flushing the Ion Sweep Cone and Ion Transfer Capillary
- Checking the Vacuum Pressure in the Ion Trap
- Cleaning the Ion Transfer Capillary and Ion Sweep Cone
- Maintaining the Internal Components of the Ion Source Interface

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. For procedures that describe how to handle a particular solvent, refer to your supplier's Material Safety Data Sheets (MSDS).

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

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 setting up the LC pump to pump a 50:50 methanol / distilled water solution through the API source.

To flush the sample transfer line, sample tube, and API probe, follow the procedure described in "Flushing the Sample Transfer Line, Sample Tube, and API Probe" on page 61.

Flushing the Ion Sweep Cone and Ion Transfer Capillary

To prevent corrosion and to maintain optimum performance of your API source, you must 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. 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. To clean the ion sweep cone and the ion transfer capillary follow the procedure described in "Flushing the Ion Sweep Cone and Ion Transfer Capillary" on page 63.

Checking the Vacuum Pressure in the Ion Trap

A blocked ion transfer capillary can cause a loss of vacuum in the ion transfer capillary-skimmer region.

❖ **To check the Convectron gauge pressure reading**

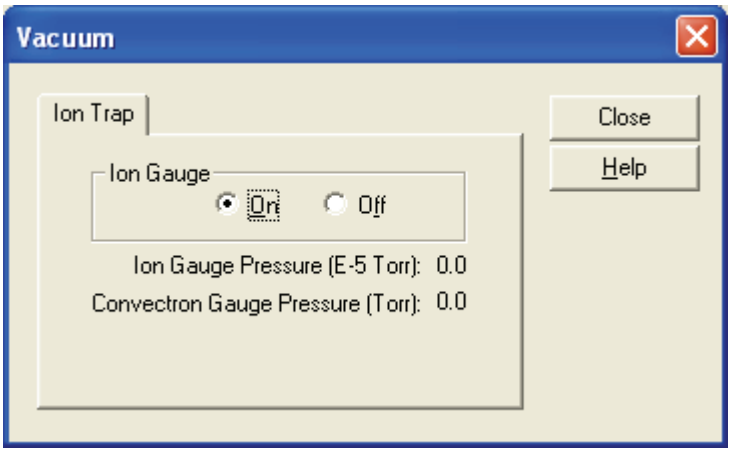
1. From the Windows XP taskbar, choose **Start > All Programs > Xcalibur > LCQ Fleet Tune**.

   The LCQ Fleet Tune window appears.

2. Choose **Setup > Vacuum**

   The Vacuum dialog box appears. See Figure 27.

Figure 27. Vacuum dialog box



Cleaning the Ion Transfer Capillary and Ion Sweep Cone

Salt buildup from buffered mobile phases or complex sample matrices or contamination from concentrated samples can block the bore of 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, a blocked ion transfer capillary is the likely cause.

The ion transfer capillary is located behind the ion sweep cone and can be easily removed for cleaning. You do not have to vent the system to remove the ion transfer capillary.

To clean the ion transfer capillary, perform the following steps:

1. Removing the Ion Transfer Capillary and the Ion Sweep Cone
2. Cleaning the Ion Transfer Capillary, Sweep Cone, and Spray Cone O-ring
3. Reinstalling the Spray Cone O-ring, Ion Transfer Capillary, and Ion Sweep Cone

Removing the Ion Transfer Capillary and the Ion Sweep Cone

❖ **To remove the ion transfer capillary and the ion sweep cone**

1. To turn off the solvent flow from the LC pump to the API source
   a. Choose **Start > Programs > Xcalibur > LCQ Fleet Tune**.

      The Tune Plus window appears.

   b. In the LCQ Fleet Tune Plus window, choose **Setup > Inlet Direct Control** (or click **AS/LC direct control**).

      The Inlet Direct Control view appears.

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

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

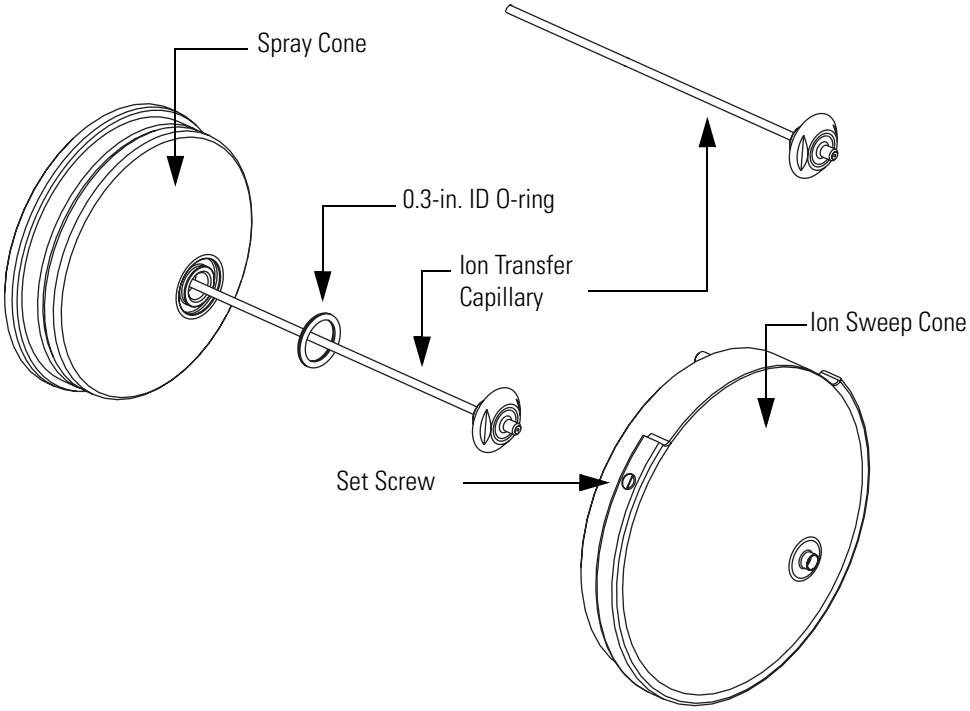
CAUTION Make sure that the LCQ Fleet electronics service switch is in the Service position before you proceed.

3. Remove the Ion Max ion source housing from the front of the MS detector as described in "Removing the Ion Max Ion Source Housing" on page 77.

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. To remove the ion sweep cone, grasp its outer ridges and pull it straight off of the API cone seal. If you cannot separate the ion sweep cone from the API cone seal, loosen the set screws on the ion sweep cone in order to remove it. See Figure 28.

Figure 28. Removing the ion sweep cone, ion transfer capillary, and 0.3-in. ID O-ring



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 the ion transfer capillary free from the ion source interface.
6. Remove the 0.3-in. ID Kalrez® O-ring (P/N 00107-12750) that is seated in the spray cone under the entrance end of the ion transfer capillary.

Cleaning the Ion Transfer Capillary, Sweep Cone, and Spray Cone O-ring

❖ **To clean the ion transfer capillary, sweep cone, and spray cone O-ring**

1. To remove contaminants, soak the ion transfer capillary in a dilute solution of nitric acid.
2. Sonicate the ion transfer capillary in distilled water.
3. Clean the ion sweep cone by wiping the inside and outside with methanol and a Kimwipe.
4. Clean the 0.3-in. ID Kalrez® O-ring with methanol.

Reinstalling the Spray Cone O-ring, Ion Transfer Capillary, and Ion Sweep Cone

❖ **To reinstall the spray cone O-ring, ion transfer capillary, and ion sweep cone**

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

CAUTION To prevent damage, be careful not to bend the ion transfer capillary. Rotate the capillary as you insert it.

2. 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.
3. Reinstall the ion sweep cone on the ion source interface.
4. Reinstall the Ion Max ion source housing on the MS detector as described in "Reinstalling the Ion Max Ion Source Housing" on page 85.

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

5. To turn on the non-vacuum system voltages, place the electronics service switch in the Electronics Normal position.

Maintaining the Internal Components of the Ion Source Interface

The ion source interface includes the ion sweep cone, ion transfer capillary, capillary heater, tube lens, and skimmer. The ion sweep cone and ion transfer capillary are not under vacuum, and you can remove them for cleaning or replacement without venting the system. For information on maintaining these parts, see Cleaning the Ion Transfer Capillary and Ion Sweep Cone on page 73 and Flushing the Ion Sweep Cone and Ion Transfer Capillary on page 72.

To clean or replace the components of the ion source interface that are under vacuum, perform the following steps:

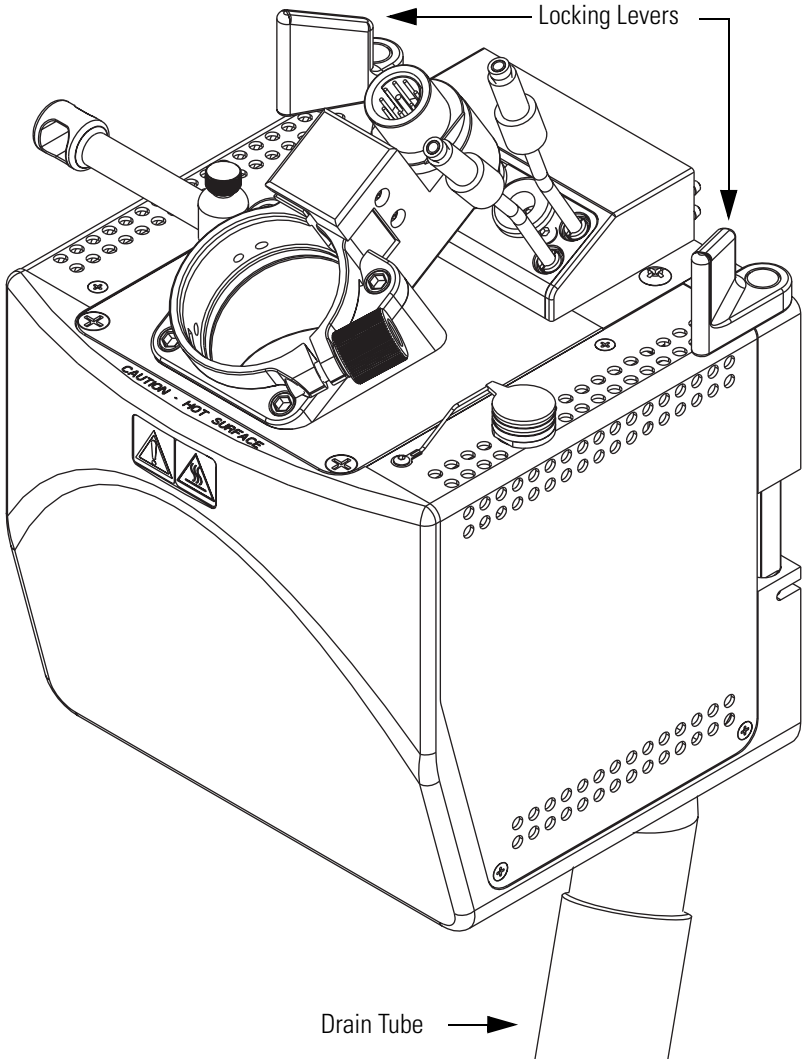
1. Removing the Ion Max Ion Source Housing
2. Removing the Ion Source Interface from the Vacuum Manifold
3. Cleaning the Tube Lens and Skimmer
4. Replacing the Ion Source Interface Components
5. Reinstalling the Ion Source Interface
6. Reinstalling the Ion Max Ion Source Housing

Removing the Ion Max Ion Source Housing

❖ **To remove the Ion Max Ion Source Housing from the front of the MS detector**

1. If you have not already done so, disconnect any liquid lines connected to the ion source housing.
2. Remove the drain tube from the ion source housing drain. See Figure 29.

Figure 29. Ion Max-S ion source



3. Rotate the ion source housing locking levers 90º to release the ion source housing from the ion source mount assembly.
4. 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.

Removing the Ion Source Interface from the Vacuum Manifold

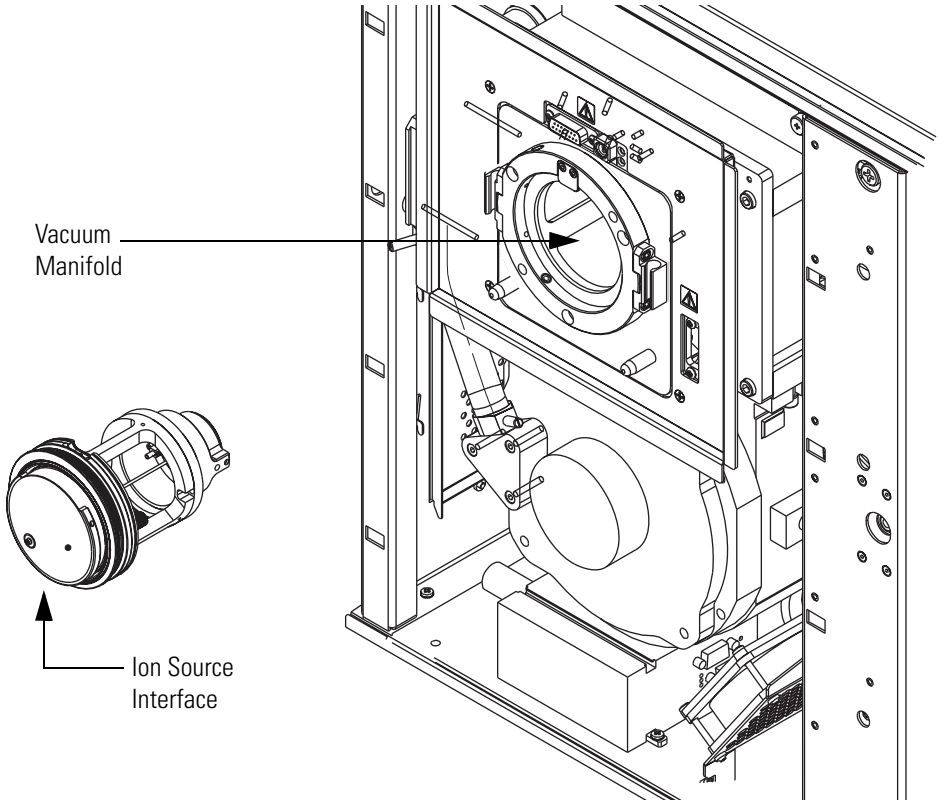
❖ **To remove the ion source interface from the vacuum manifold**

1. Shut down and vent the system as described in "Shutting Down the System Completely" on page 113. Wait several minutes for the LCQ Fleet to vent.
2. Ensure that you have removed the LCQ Fleet from line power by unplugging its power cord.

CAUTION Make sure to unplug the LCQ Fleet power cord before you proceed.

3. Grasp the ridges on either side of the ion source interface and carefully pull it free from the vacuum manifold.
4. Place the ion source interface on a clean surface.

Figure 30. Removing the ion source interface from the vacuum manifold



Cleaning the Tube Lens and Skimmer

Chemicals that accumulate on the surfaces of the tube lens and skimmer form 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.

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

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

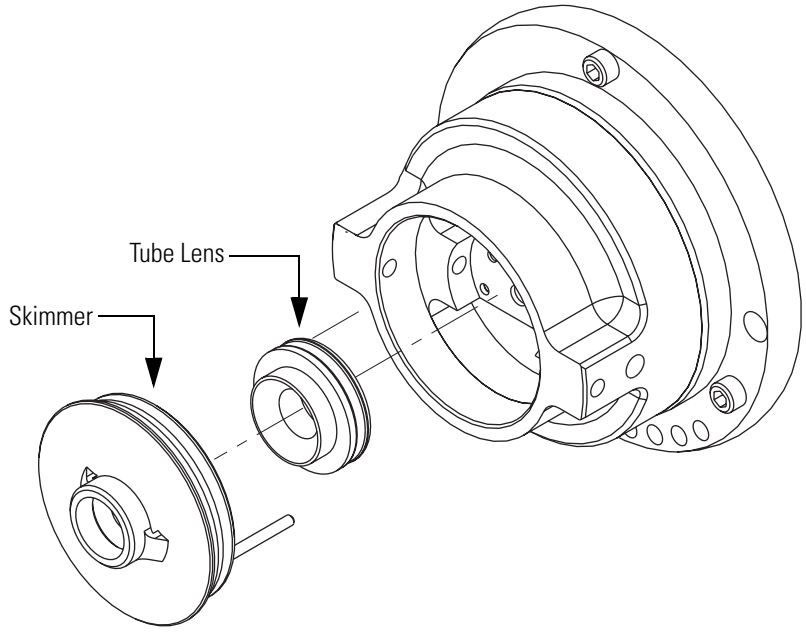
❖ To clean the tube lens and skimmer

1. To remove the skimmer, carefully pull it free from the rear of the ion source interface. Note the orientation of the skimmer.

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

2. To remove the tube lens, carefully pull it free from the rear of the ion source interface. Note the orientation of the tube lens.

Figure 31. Removing the skimmer and the tube lens from the back of the ion source interface



3. Clean the tube lens inside and out with a cotton-tipped applicator (swab) soaked in HPLC-grade methanol.

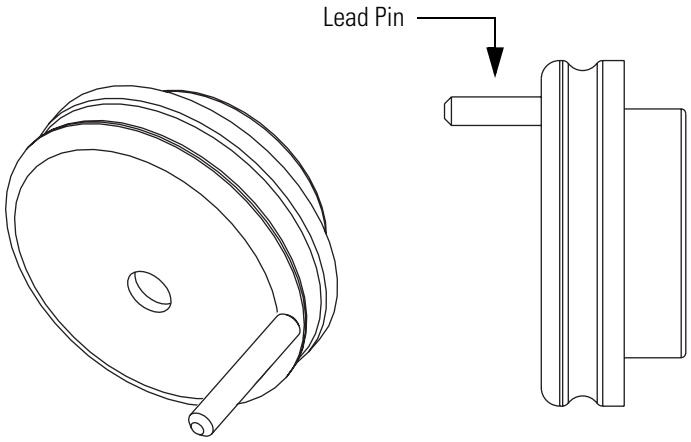
4. Clean the skimmer inside and out with HPLC-grade methanol and a cotton-tipped applicator (swab).

   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.

5. To reinstall the tube lens in the ion source interface

   a. Orient the tube lens so that the lead pin aligns with the socket. See Figure 32.

   Figure 32. View of the tube lens, showing the orientation of the lead pin



   b. Push the tube lens until it snaps into place.

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

6. To reinstall the skimmer in the ion source interface

   a. Orient the skimmer so that the lead pin aligns with the socket.

   b. Push the skimmer until it snaps into place.

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

Replacing the Ion Source Interface Components

You must replace the capillary heater assembly (P/N 97055-60176) as a unit.

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.

❖ To remove the capillary heater assembly

1. To remove the ion transfer capillary, turn it counterclockwise until you can pull it free from the ion source interface.
2. Disconnect the capillary heater cable.
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.

❖ To install a capillary heater assembly

1. Connect the capillary heater mount to the ion source interface housing.
2. Connect the grounding wire.
3. Connect the capillary heater cable.
4. Insert the ion transfer capillary into the ion source interface.

To replace other ion source interface components, refer to the exploded diagrams shown in Figure 33, Figure 34, and Figure 35.

Figure 33. Exploded view of the ion source interface (front)

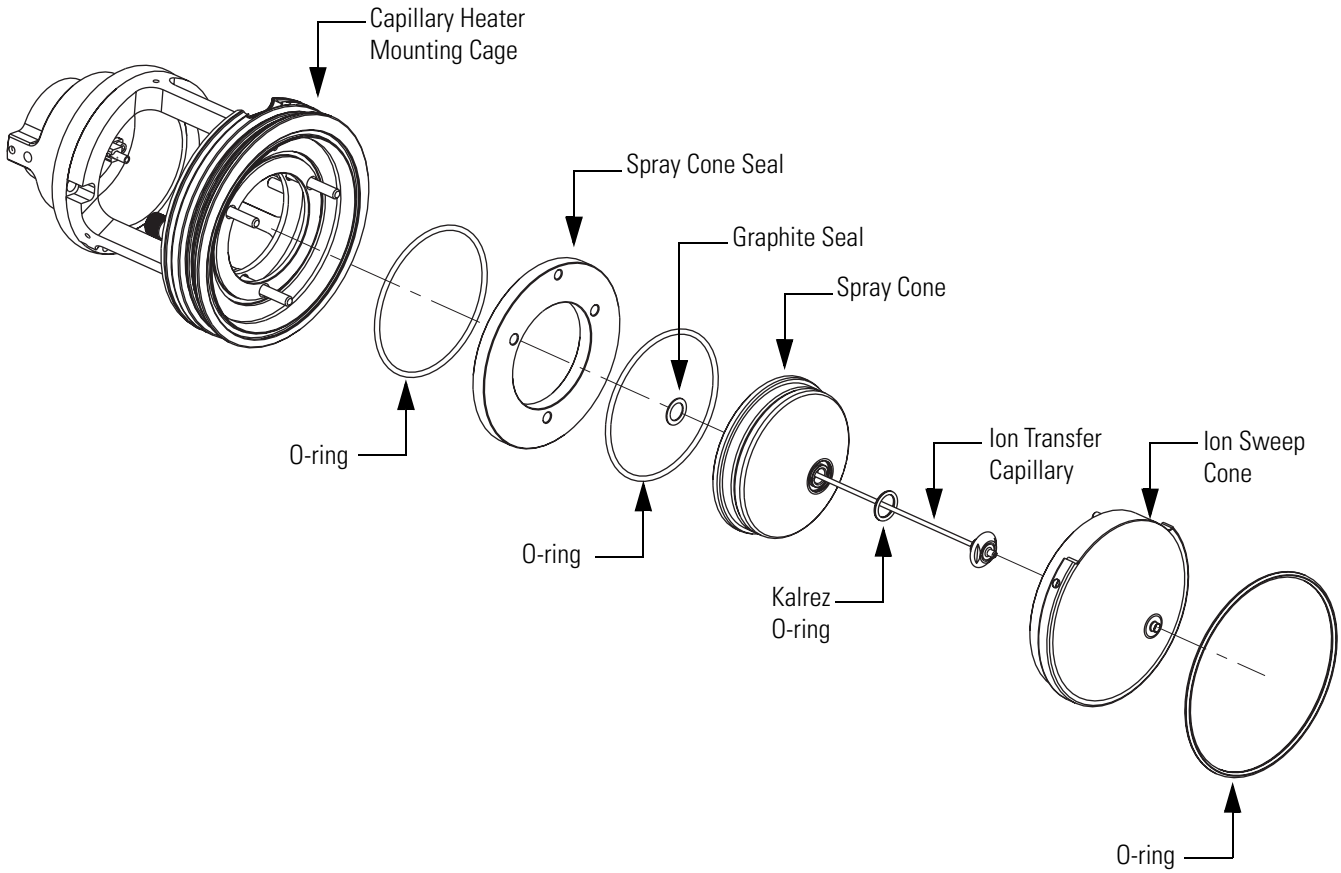


Figure 34. Exploded view of the ion source interface (rear)

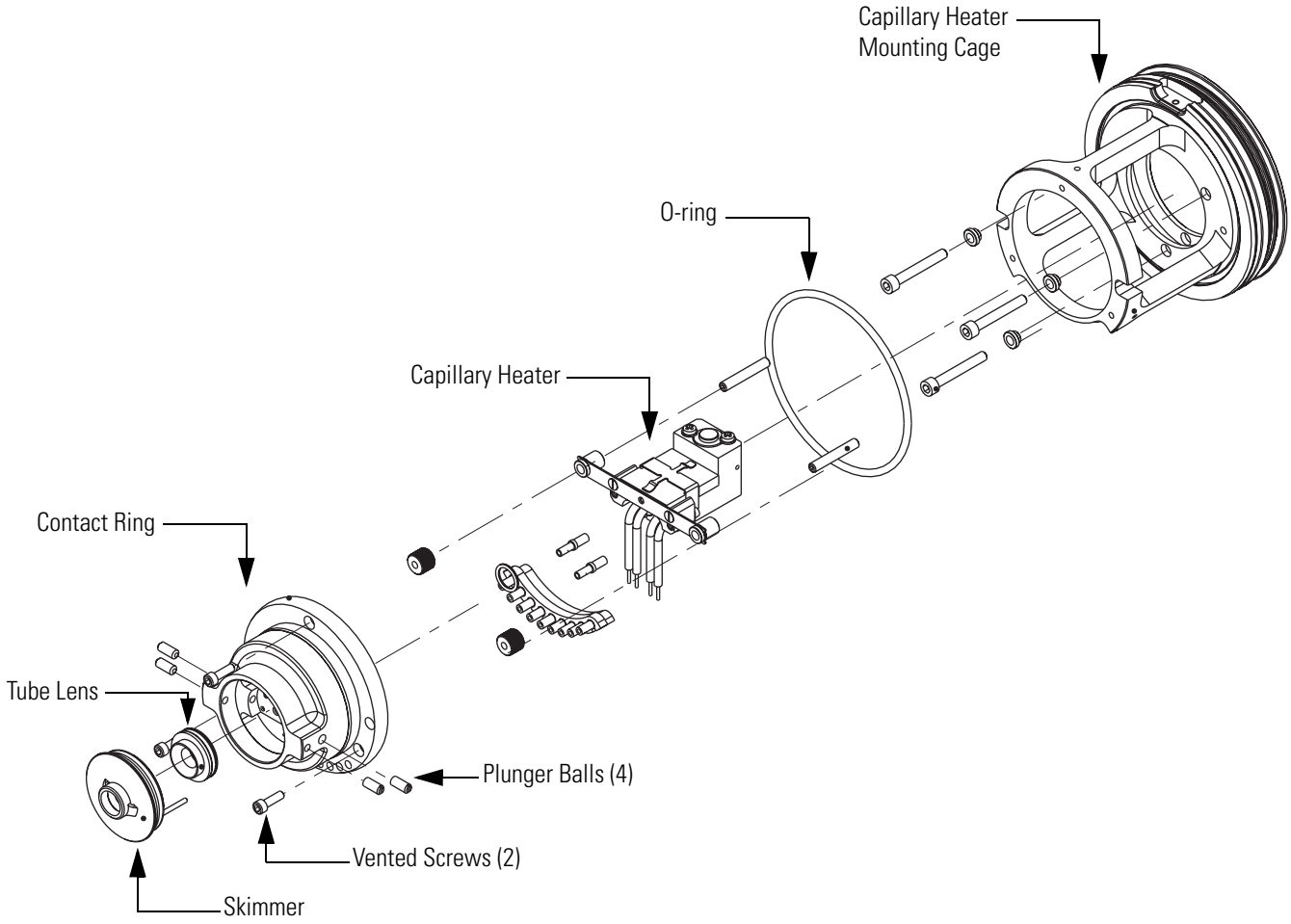
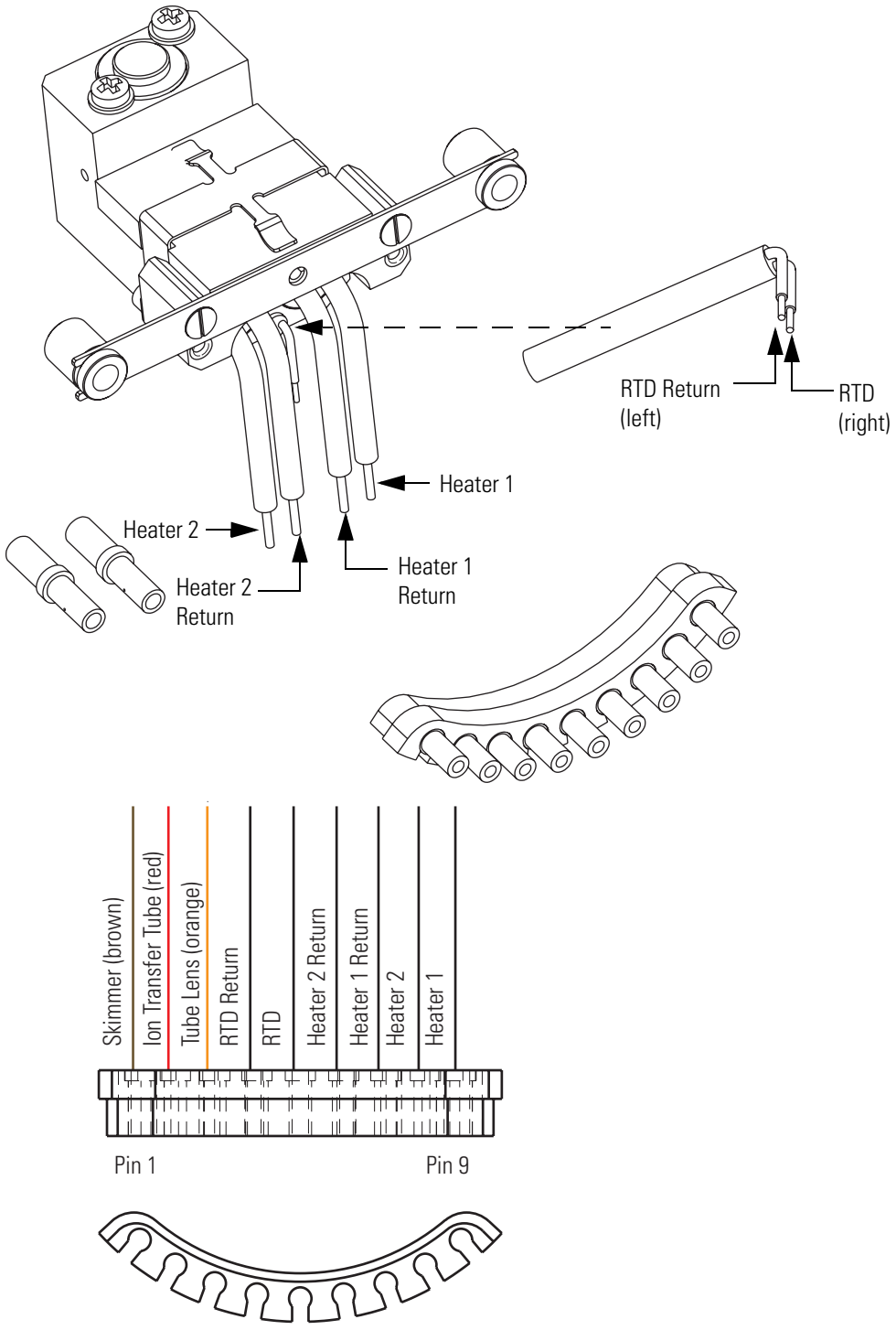


Figure 35. Capillary heater assembly and wiring diagram for the ion source interface



Reinstalling the Ion Source Interface

❖ To reinstall the ion source interface

1. Orient the ion source interface as shown in Figure 30.
2. Carefully insert the ion source interface into the vacuum manifold until it is seated in the Q00 RF lens.

Reinstalling the Ion Max Ion Source Housing

❖ To reinstall the Ion Max ion source housing

1. Carefully align the two guide pin holes on the rear of the source housing (see Figure 36) with the ion source housing guide pins on the mass spectrometer (see Figure 37), and carefully press the ion source housing onto the ion source mount.
2. Rotate the ion source housing locking levers 90 degrees to lock the ion source housing onto the ion source mount assembly.

Figure 36. Rear view of the Ion Max-S source housing

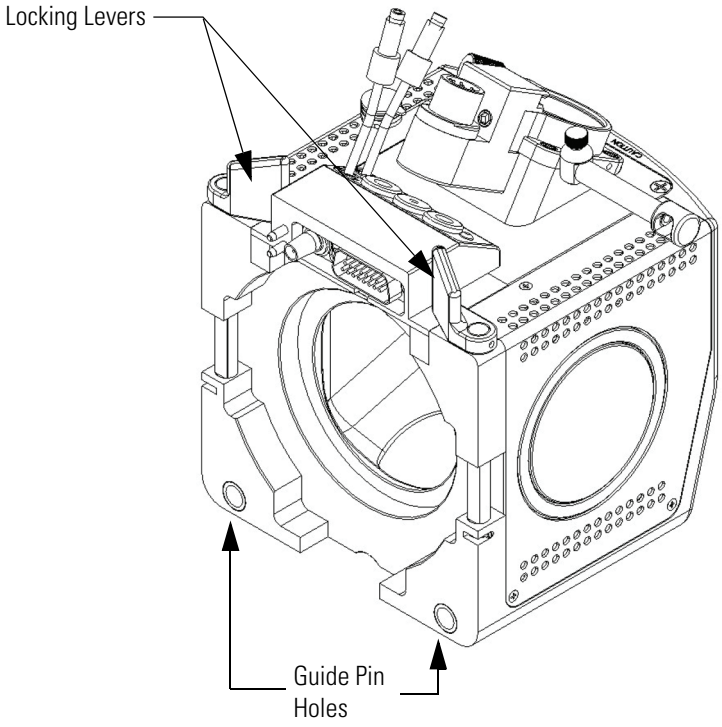
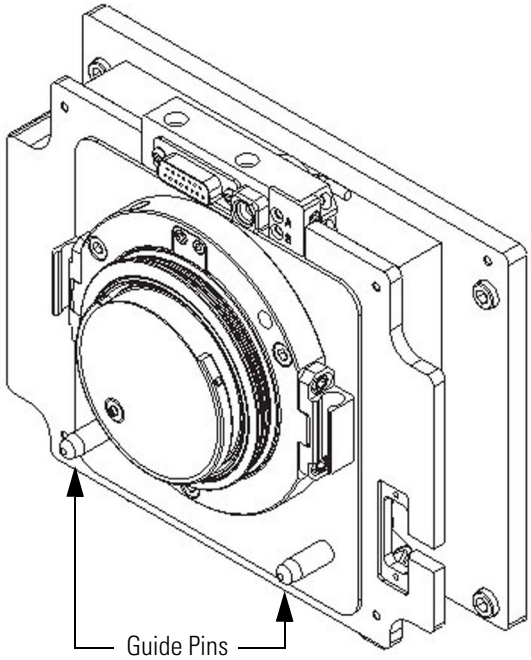


Figure 37. Ion source mount



3. To reinstall the source drain tube and restart the 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, and vent the waste container to a fume exhaust system.

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.

CAUTION Your laboratory must be equipped with at least two independent fume exhaust systems. Route the (blue) forepump exhaust tubing to the first dedicated fume exhaust system. Route the drain tube from the Ion Max ion source to a waste container. Vent this waste container to the second dedicated fume exhaust system.

CAUTION Do not vent the Ion Max ion source drain tube (or any vent tube connected to the waste container) to the same fume exhaust system to which you have connected the forepump. The analyzer optics can become irreversibly contaminated with pump oil residue if the Ion Max ion source drain tube and the blue forepump exhaust tubing are connected to the same fume exhaust system.

   c. Start the system as described in "Starting the System after a Complete Shutdown" on page 115.

Cleaning the Q00-L0 RF Lens

Chemicals that accumulate on the surfaces of the Q00 segments and lens L0 form an insulating layer that can modify the electrical fields that control ion transmission. Therefore, clean ion guide components are essential to the performance of the instrument. The Q00 segments 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 RF lens components, perform the following steps:

1. Removing the Q00-L0 RF Lens from the Vacuum Manifold
2. Disassembling the Q00-L0 RF Lens
3. Cleaning the Q00-L0 RF Lens Components
4. Reassembling the Q00-L0 RF Lens
5. Reinstalling the Q00-L0 RF Lens

Removing the Q00-L0 RF Lens from the Vacuum Manifold

Before you remove the Q00-L0 RF Lens from the vacuum manifold, you must shut down the MS detector, and then remove the ion source and the ion source interface.

❖ To remove the Q00-L0 RF lens

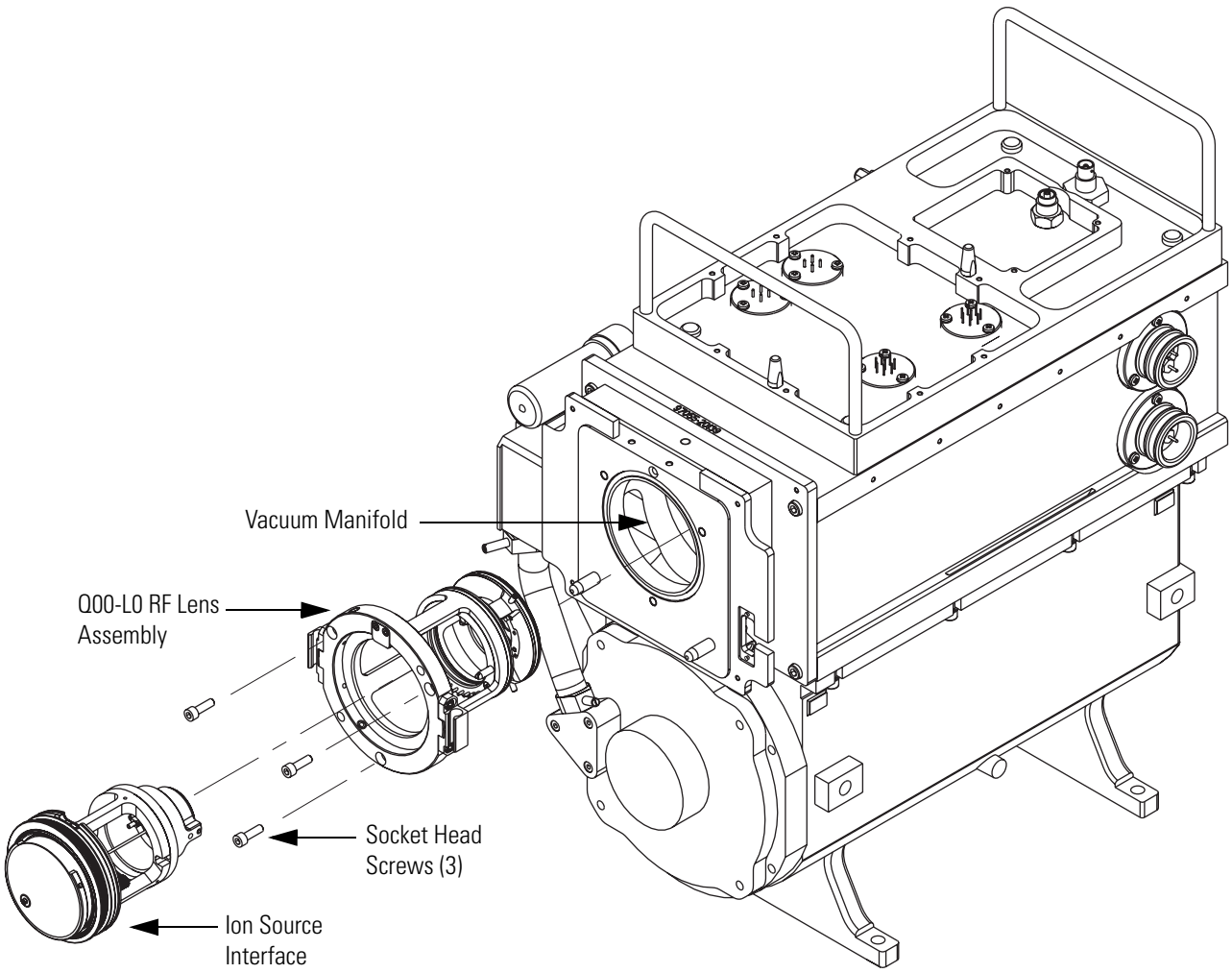
1. Shut down and vent the system as described in "Shutting Down the System Completely" on page 113.

CAUTION Make sure to unplug the LCQ Fleet power cord before you proceed.

2. Remove the Ion Max ion source from the front of the MS detector as described in Removing the Ion Max Ion Source Housing on page 77.
3. Remove the ion source interface as described in "Removing the Ion Source Interface from the Vacuum Manifold" on page 78.
4. Reach into the opening in the vacuum manifold (where the ion source interface was) and disconnect the electrical connector to the Q00-L0 RF lens.

5. Loosen the three mounting bolts that hold the Q00-L0 RF lens housing to the vacuum manifold. See Figure 38.
6. Carefully remove the Q00-L0 RF lens assembly and place it on a clean surface.

Figure 38. Q00-L0 RF lens assembly removal

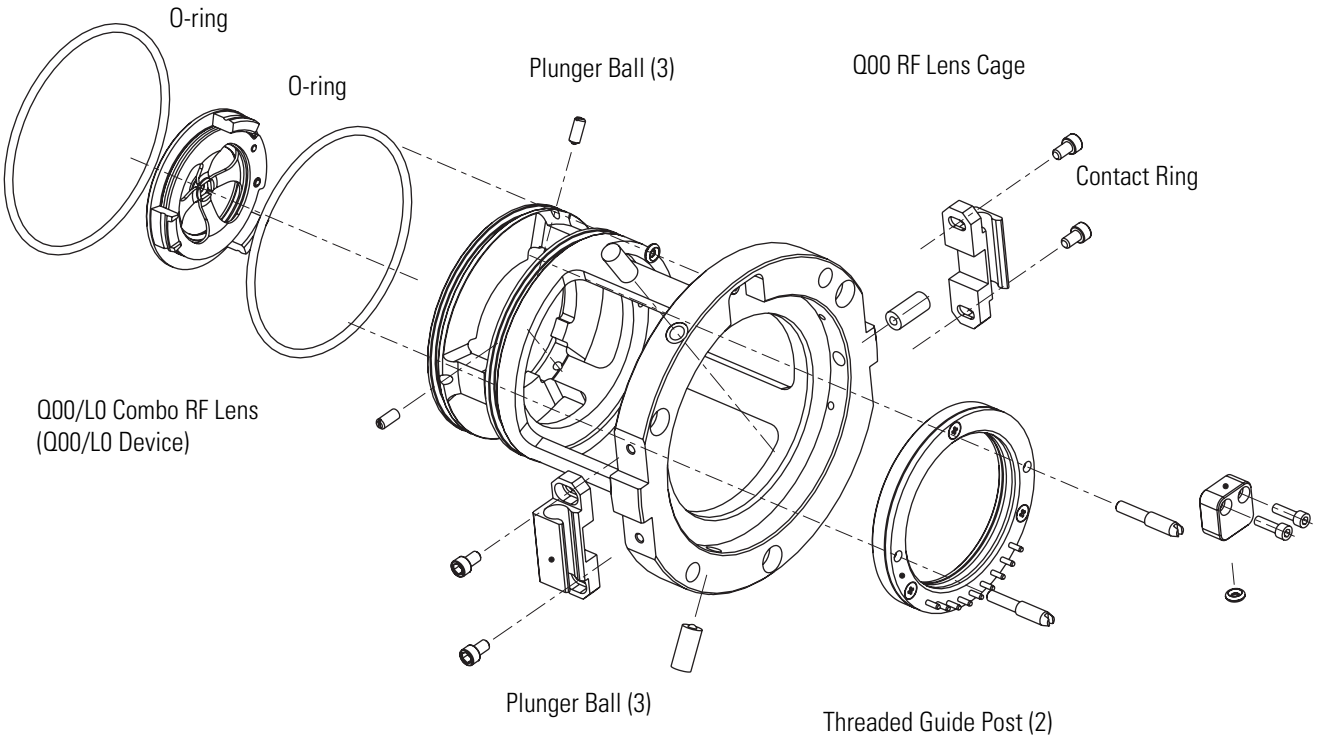


Disassembling the Q00-L0 RF Lens

❖ **To disassemble the Q00-L0 RF lens**

1. Prepare a clean work area by covering the area with lint-free paper.
2. Put on clean gloves before you handle the Q00-L0 RF lens components.
3. Remove the Q00-L0 device from the rear of the Q00 RF lens cage. The Q00-L0 device is secured to the Q00 RF lens cage by plunger balls. Figure 39 shows the location of the Q00-L0 RF lens components.

Figure 39. Exploded view of the Q00-L0 RF lens



Cleaning the Q00-L0 RF Lens Components

❖ **To clean the Q00-L0 RF lens**

1. With a soft toothbrush or lint-free swab, scrub the contaminated 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, and 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.

Reassembling the Q00-L0 RF Lens

❖ **To reassemble the Q00-L0 RF lens**

Insert the Q00-L0 device through the rear of the Q00 RF lens cage until it is seated in the cage.

Reinstalling the Q00-L0 RF Lens

❖ **To reinstall the Q00-L0 RF lens in the vacuum manifold**

1. Ensure that the two 2.148-in. O-rings (P/N 00107-15542) are properly installed on the back of the Q00 RF lens cage.
2. Orient the Q00-L0 RF lens assembly as shown in Figure 38 on page 88.
3. Carefully insert the Q00-L0 RF lens assembly into the vacuum manifold.
4. Reconnect the electrical connections.
5. Reinstall the ion source interface as described in "Reinstalling the Ion Source Interface" on page 85.
6. Reinstall the Ion Max ion source housing as described in Reinstalling the Ion Max Ion Source Housing on page 85.
7. Start up the system as described in "Starting the System after a Complete Shutdown" on page 115.

Cleaning the Q0 and Q1 Ion Guides

Chemicals that accumulate on the surfaces of the Q0 and Q1 ion guides form an insulating layer that can modify the electrical fields that control ion transmission. Therefore, clean ion guide components are essential to the performance of the instrument. The Q0 and Q1 ion guides require cleaning less frequently than the Q00 RF lens. The frequency of cleaning depends on the type and quantity of the compounds that you analyze.

To clean or replace Q0 and Q1 ion guide components, perform the following steps:

1. Removing the Top Cover of the MS Detector
2. Removing the Top Cover Plate of the Vacuum Manifold
3. Removing the Q0 and Q1 Ion Guides
4. Cleaning the Q0 and Q1 Ion Guides
5. Reinstalling the Q0 and Q1 Ion Guides
6. Cleaning the Ion Detection System
7. Reinstalling the Top Cover Plate of the Vacuum Manifold
8. Reinstalling the Top Cover of the MS Detector

Removing the Top Cover of the MS Detector

❖ **To remove the top cover of the MS detector**

1. Shut down and vent the system as described in "Shutting Down the System Completely" on page 113.

CAUTION Make sure to unplug the LCQ Fleet power cord before you proceed.

2. Open the front door of the MS detector by loosening the Allen screw on the right side of the door with an Allen wrench.
3. 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.
4. Slide the top cover back by about 1.2 cm (0.5 in.).
5. With one hand under the center of the top cover, lift the top cover up and away from the MS detector.

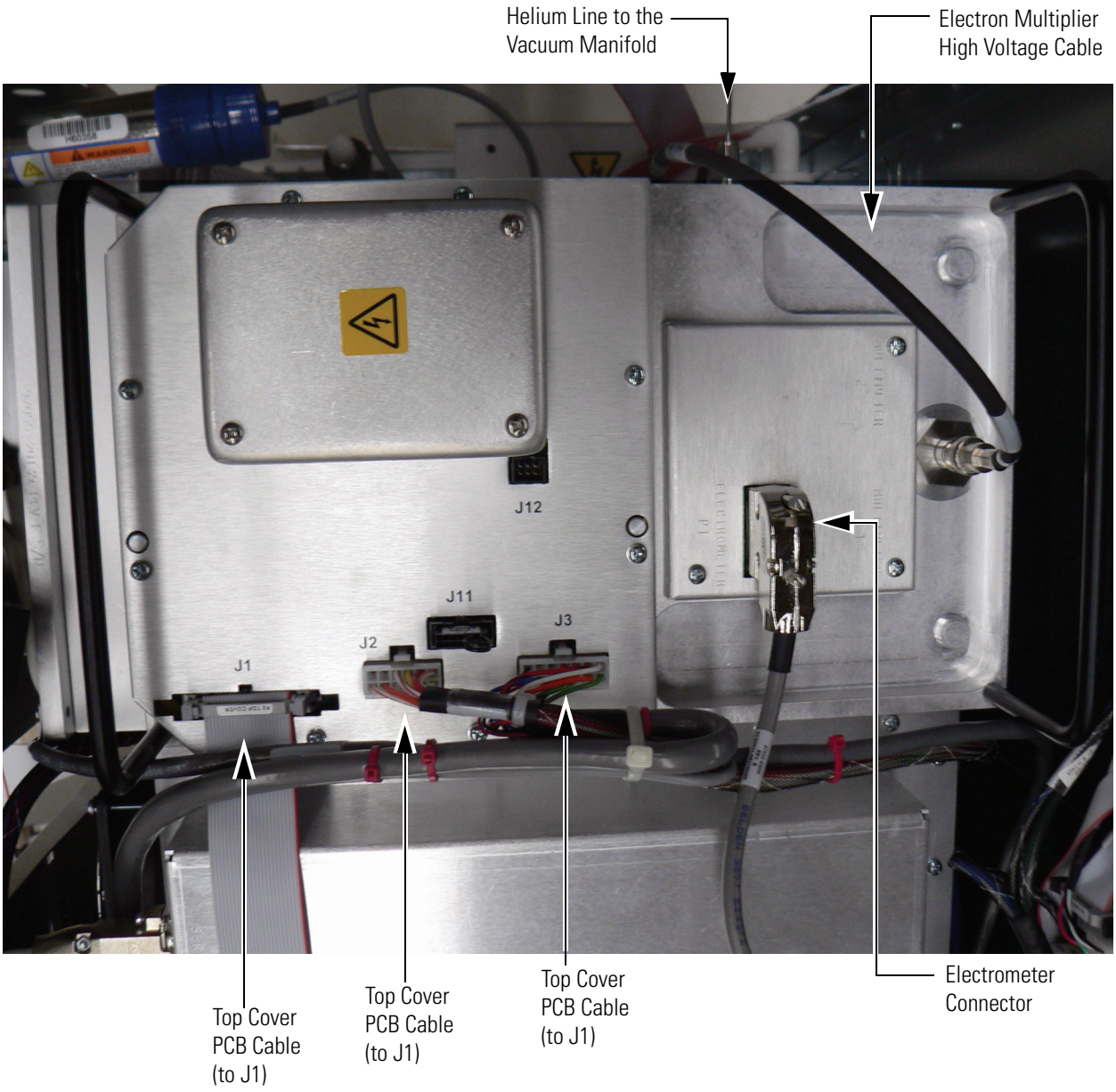
Removing the Top Cover Plate of the Vacuum Manifold

You must 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. Five cables are connected to the top cover plate and a helium gas line Swage-lok® fitting. See Figure 40.

❖ To remove the top cover plate

1. Disconnect the electron multiplier high voltage coaxial cable that originates 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. Disconnect the helium tube from the top cover.
5. 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.
6. Cover the opening in the top of the vacuum manifold with a large, lint-free tissue.

Figure 40. Electrical and helium connections to the top cover of the vacuum manifold



Removing the Q0 and Q1 Ion Guides

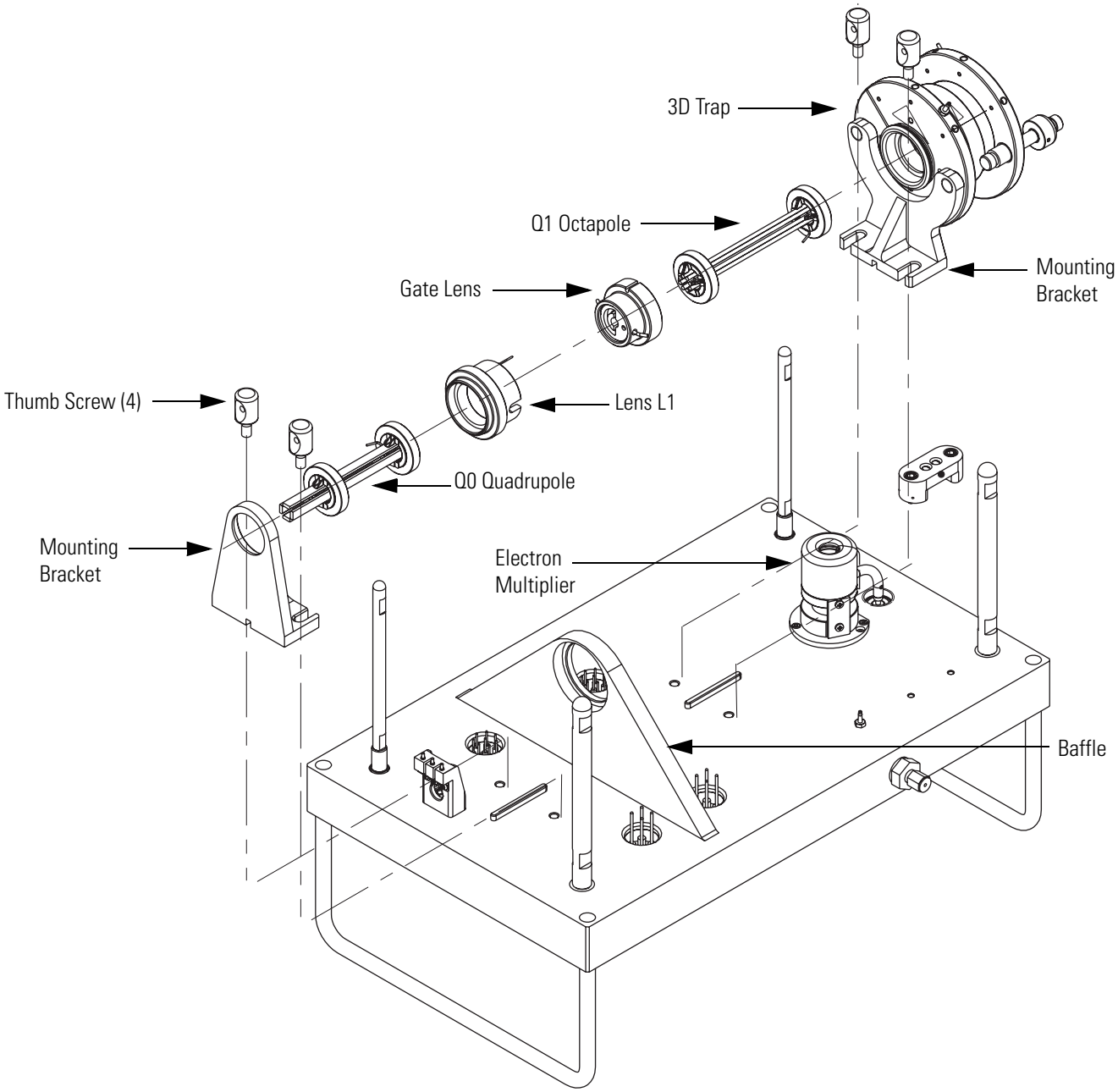
❖ **To remove the Q0 and Q1 ion guides from the top cover plate**

1. Prepare a clean work area by covering the area with lint-free paper. Place each part on the paper as you remove it.
2. To handle the ion guides, wear clean, lint-free, nylon or cotton gloves.

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

3. Disconnect the electrical leads to the Q0 quadrupole, lens L1, gate lens, Q1 octapole, and ion trap.
4. Disconnect the Teflon tube from the nipple located entrance end cap electrode of the ion trap.
5. Holding 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. Slide the 3D trap back. See Figure 41.
6. Remove the Q0 quadrupole and lens L1.
7. Hold the Q1 octapole and gate lens with one hand; loosen and remove the two thumb screws that hold the ion trap mounting bracket to the top cover plate of the vacuum manifold. See Figure 41.
8. Remove the Q1 octapole and gate lens.

Figure 41. Exploded view of the Q0 and Q1 ion guides



Cleaning the Q0 and Q1 Ion Guides

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.

❖ **To remove contamination from the Q0 quadrupole, Q1 octapole, lens L1, and the gate lens**

1. With a soft tooth brush or lint-free swab, scrub the ion guide part with a solution of detergent and water.

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

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 seconds.

   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, and 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.

Reinstalling the Q0 and Q1 Ion Guides

Two adjustable mounting brackets hold the Q0 and Q1 ion guides in position on the top cover plate of the vacuum manifold. See Figure 41.

❖ **To re-install the Q0 and Q1 ion guides on the top cover plate**

Note To handle the ion guides, wear clean, lint-free, nylon or cotton gloves.

1. To install the Q0 ion guide
   a. Insert lens L1 into the opening in the baffle (Figure 41).

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.

2. To install the Q1 ion guide

   a. Insert the gate lens into the opening in the baffle (Figure 41).

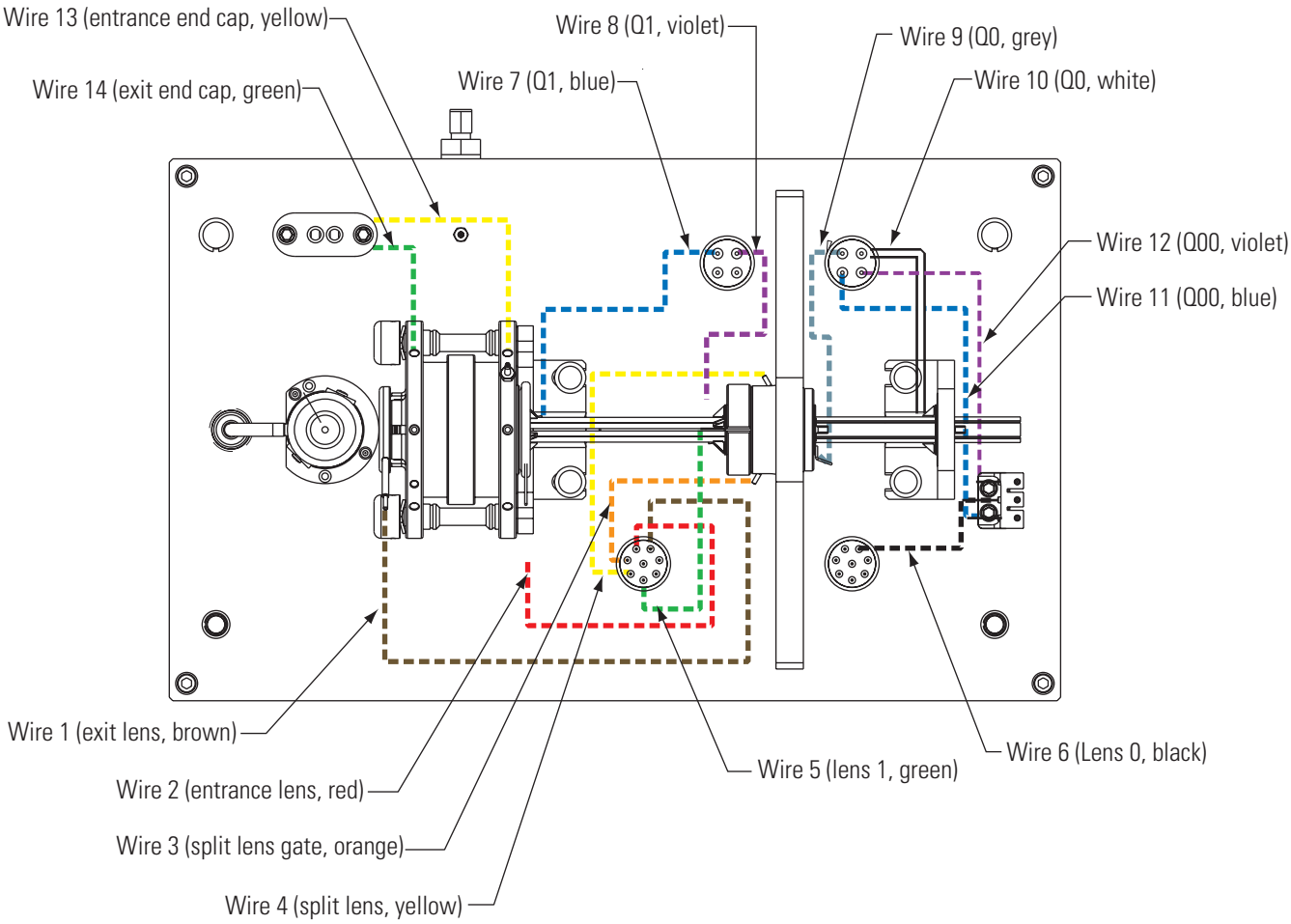
   b. With one hand, hold the Q1 octapole against the gate lens; with the other hand, install the ion trap mounting bracket so that the octapole is held between the mounting bracket and the gate lens.

   c. Tighten the two thumb screws that hold the Q1 ion guide mounting bracket to the top cover plate.

3. Reconnect the electrical leads to the Q0 quadrupole, lens L1, gate lens, Q1 octapole, and ion trap, according to the diagram shown in Figure 42.

4. Check all leads to ensure that they are secure and that they are attached to the proper electrodes.

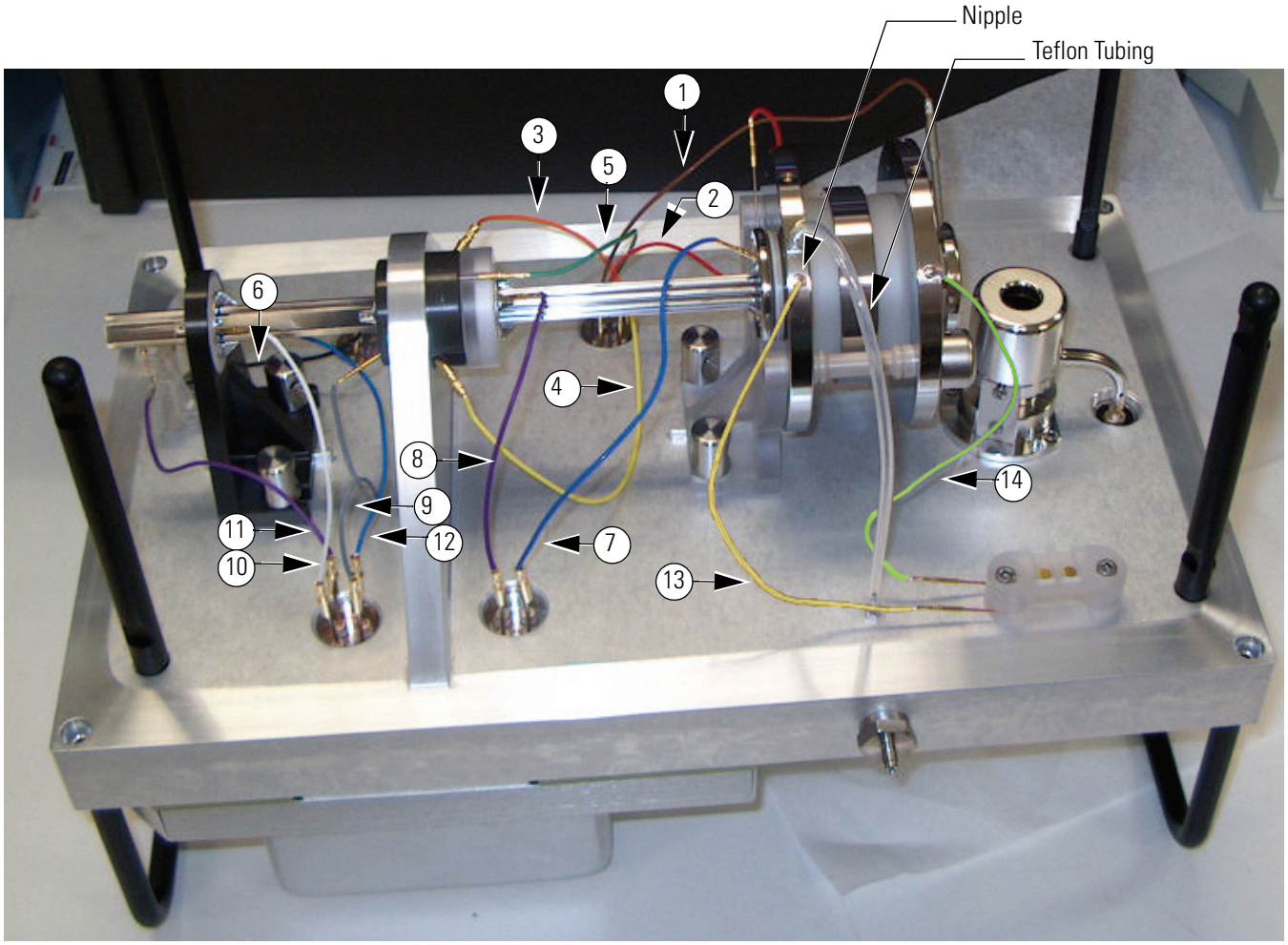
Figure 42. Wiring diagram for the Q0 and Q1 ion guides



5. Slide the tubing for the helium damping gas onto the nipple located on the entrance end cap electrode of the ion trap.

   Figure 43 shows the connection of the tubing for the helium damping gas to the nipple on the ion trap and the wires to the connected to the Q0 and Q1 ion guides. The numbered wires in the photograph correspond to the numbered wires shown in the schematic (Figure 42).

Figure 43. View of the tubing that connects the helium damping gas to the ion trap



Cleaning the Ion Detection System

To keep the conversion dynode and electron multiplier of the ion detection system dust free, clean these components whenever you remove the top cover plate of the vacuum manifold. To clean the conversion dynode and electron multiplier, blow off the dust with a clean, dry gas such as nitrogen. Do not use freon gas.

Note 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.

Reinstalling the Top Cover Plate of the Vacuum Manifold

❖ **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 by its two handles and turn it over. Orient the top cover plate so 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, and then 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.
4. Ensure that the cover plate is seated properly on the vacuum manifold.
5. Reconnect the three cables to the top cover PCB. See Figure 40.
6. Reconnect the electron multiplier high voltage coaxial cable that comes from the electron multiplier power supply.
7. Reconnect the electrometer cable to the electrometer PCB.
8. Reconnect the helium gas line.

Reinstalling the Top Cover of the MS Detector

❖ **To reinstall the top cover of the MS detector**

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 so that the front of the cover is about 1.2 cm (0.5 in.) behind the front of the MS detector.
3. Slide the cover forward 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 screw on the right side of the door.
6. Start up the system as described in "Starting the System after a Complete Shutdown" on page 115.

Maintaining the Mass Analyzer

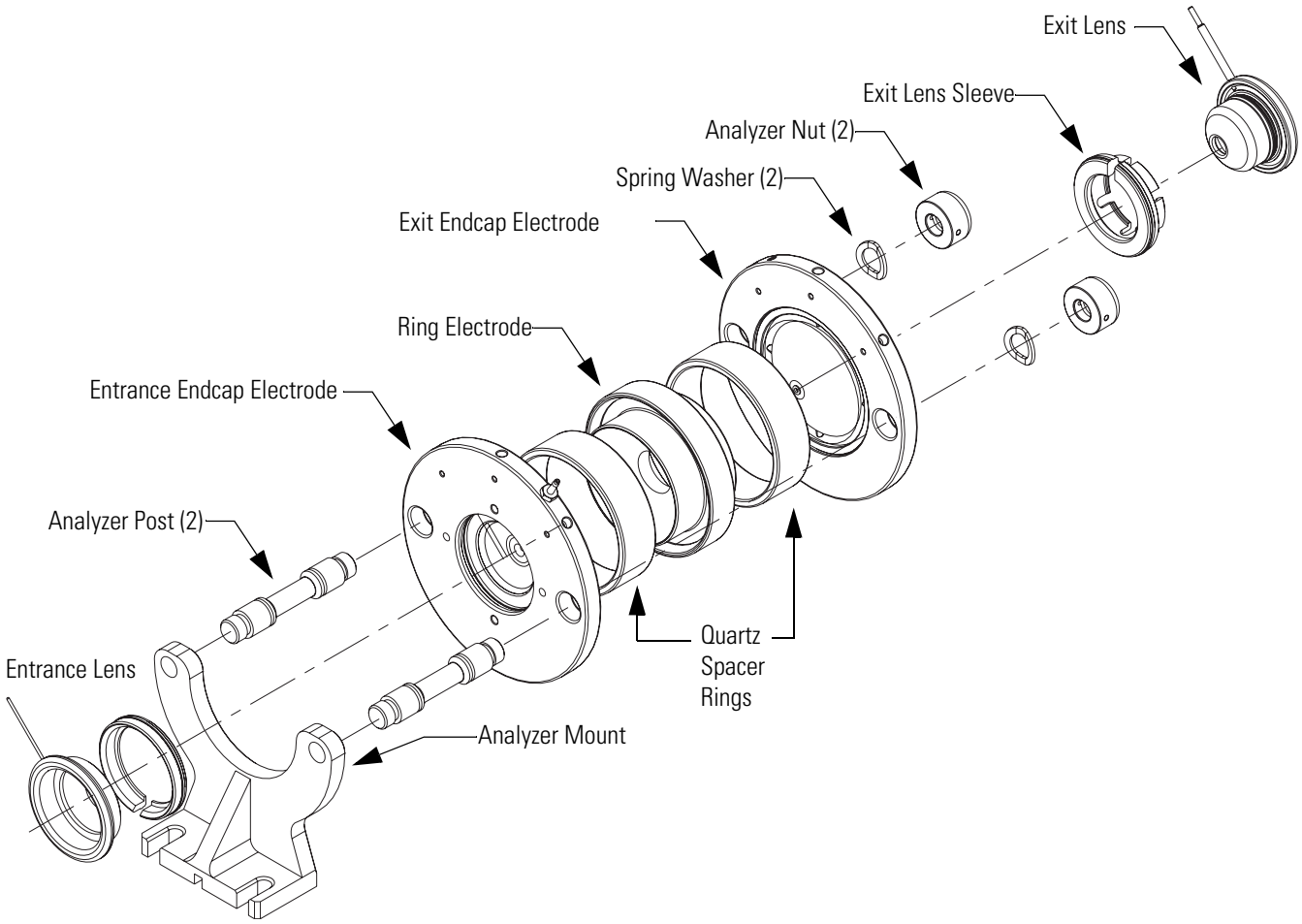
Although the mass analyzer very rarely requires cleaning, you can clean it by performing the following steps:

1. Removing the Mass Analyzer
2. Disassembling the Mass Analyzer
3. Cleaning the Mass Analyzer Parts
4. Reassembling the Mass Analyzer
5. Reinstalling the Mass Analyzer

Removing the Mass Analyzer

The ion optics and mass analyzer are mounted on a plastic mount on the underside of the top cover plate of the vacuum manifold. See Figure 44 for the location of the ion optics and mass analyzer components.

Figure 44. Mass analyzer exploded view



❖ To remove the mass analyzer from the MS detector

IMPORTANT Wear clean, lint-free, nylon or cotton gloves when you handle the mass analyzer and its components.

1. Disconnect the electrical leads to the entrance lens, entrance endcap electrode, exit endcap electrode, and the exit lens of the mass analyzer. See Figure 42 on page 98.
2. Disconnect the tubing for the helium damping gas from the nipple on the exit endcap electrode by pulling the line free from the nipple. See Figure 43 on page 99.
3. Holding the mass analyzer with one hand, loosen the two thumb screws that hold the analyzer mount to the top cover.
4. With one hand holding the mass analyzer and the other hand holding the octapole, slide the mass analyzer away from the baffle on the top cover plate. Take care not to touch the electron multiplier with the mass analyzer, as doing so could damage the electropolished surface of the electron multiplier. Take care not to drop the octapole, as doing do could damage it.

Disassembling the Mass Analyzer

Figure 44 on page 101 shows the location of the ion optics and mass analyzer components.

❖ To disassemble the mass analyzer

1. Remove the entrance lens by pulling the entrance lens out of the entrance lens sleeve.
2. Remove the entrance lens sleeve by squeezing the sleeve and pulling it out of the recess in the entrance endcap electrode.
3. Remove the exit lens by pulling it out of the exit lens sleeve. Use the connector pin to aid in pulling off the lens.
4. Remove the exit lens sleeve by squeezing the sleeve and pulling it out of the recess in the exit endcap electrode.
5. Unscrew and remove the two nuts from the posts.
6. Remove the two spring washers from the posts.
7. Remove the exit endcap electrode from the posts.
8. Remove the two spacer rings and the ring electrode.
9. Remove the entrance endcap electrode from the posts.

Cleaning the Mass Analyzer Parts

Use the following procedure to remove contamination from the ion optics and mass analyzer parts. Clean each part in turn. After cleaning, place each part on a clean, lint–free surface.

CAUTION Do not chip, scratch, or break the spacer rings of the mass analyzer. Take care not to bump or jar the octapole. Do not place the octapole in an ultrasonic cleaner.

Note When you clean the ion optics and mass analyzer parts, pay particular attention to the inside surfaces.

❖ **To remove contamination from the mass analyzer parts**

1. With a soft tooth brush or lint-free swab, scrub the ion optics or mass analyzer part with a solution of detergent and water.

CAUTION Do not use aluminum oxide to clean the ion optics or the mass analyzer. Doing so removes the XXX.

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 seconds.

   Tip You can use an ultrasonic bath to clean the ring electrode, end caps, and lens.

5. Wearing clean, lint-free, nylon or cotton gloves, do the following:
   a. Remove the part from the methanol bath
   b. Rinse the part thoroughly with fresh methanol.
   c. Dry the part with a rapid stream of nitrogen gas.
   d. Inspect each part for contamination and dust. If necessary, repeat the cleaning procedure.

Reassembling the Mass Analyzer

Figure 44 on page 101 shows the location of the ion optics and mass analyzer components.

IMPORTANT Wear clean, lint-free, nylon or cotton gloves when you handle the mass analyzer and its components.

❖ To reassemble the mass analyzer

1. Wearing clean, lint-free, nylon or cotton gloves, reinstall the entrance endcap electrode
   a. Slide the entrance endcap electrode onto the analyzer posts.
   b. Check the following:
      - The convex surface of the electrode faces away from the analyzer mount.
      - The opening in the electrode for the pin on the end of the electrical lead faces away for the top cover plate (when the analyzer mount is installed on the top cover plate), slide the entrance endcap electrode onto the analyzer posts.

CAUTION Handle the quartz spacer rings carefully. Do not scrape the spacer rings against any metal surfaces. Metal deposits on the surfaces of the spacer rings might cause potentially damaging RF voltage, arcing across the spacer rings to the endcaps. Do not overtighten the mass analyzer nuts.

2. Place a quartz spacer ring into the groove in the entrance endcap electrode.
3. Reinstall the ring electrode onto the quartz spacer ring so that the spacer ring is held securely between the electrodes. The orientation of the ring electrode is unimportant.
4. Reinstall the second quartz spacer ring into the groove in the ring electrode.
5. To reinstall the exit endcap electrode
   a. Slide the exit endcap electrode onto the analyzer posts so that the quartz spacer ring is held in place between the ring electrode and the exit endcap electrode.
   b. Check the following:
      - The electrode is oriented with the convex surface facing the spacer ring.
      - The damping gas nipple points away from the top cover plate when the analyzer mount is installed on the top cover plate.
6. Inspect the mass analyzer assembly. Ensure that all the parts are aligned properly and that they all fit together snugly.
7. Reinstall the spring washers on the analyzer posts.
8. Reinstall the analyzer nuts onto the analyzer posts and tighten the nuts by hand until they are finger tight. Do not overtighten the nuts.

9. Squeeze the exit lens sleeve and insert it into the recess in the exit endcap electrode. See Figure 44 on page 101 for the proper orientation of the exit lens sleeve.
10. Insert the exit lens into the exit lens sleeve so that the lead pin on the exit lens points in the same direction as the 8-pin feedthrough when the analyzer mount is installed on the top cover plate. Make sure that the exit lens lead pin does not contact the nut on the end of the mass analyzer post.
11. Insert the entrance lens sleeve so that the lead pin on the entrance lens points in the same direction as the 8-pin feedthrough when the analyzer mount is installed on the top cover plate.

Reinstalling the Mass Analyzer

❖ **To reinstall the mass analyzer**

IMPORTANT Wear clean, lint-free, nylon or cotton gloves when you handle the mass analyzer and its components.

1. Wearing clean, lint-free, nylon or cotton glove, insert the octapole into the gate lens and support it with your hand. See Figure 41 on page 95.
2. With your other hand, slide the mass analyzer assembly so that the octapole mates with the front lens.
3. Secure the analyzer mount to the baffle with the two thumb screws.
4. Inspect the ion optics. Ensure that all the parts are aligned properly and that they all fit together snugly.
5. Reconnect all the electrical leads. See Figure 42 on page 98.
6. Reconnect the damping gas line to the nipple on the entrance endcap electrode.

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

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. Heat, electron flow (which produces internal heat), air (which causes oxidation and arcing) and water (which causes arcing) decrease the lifetime of the cathode.

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

- Excessive noise in the mass spectrum

- Inability of the multiplier gain calibration procedure to achieve a gain of 4×10^5 electrons per ion with an electron multiplier voltage less than or equal to 2.5 kV

To check the current value of the electron multiplier voltage, choose **Setup > Ion Detection System** in Tune Plus window to open the Ion Detection System dialog box.

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

❖ To replace the electron multiplier assembly

1. Shut down and vent the system as described in "Shutting Down the System Completely" on page 113.

CAUTION Make sure to unplug the LCQ Fleet power cord before you proceed.

2. Remove the top cover of the MS detector as described in "Removing the Top Cover of the MS Detector" on page 91.
3. Remove the top cover plate of the vacuum manifold as described in "Removing the Top Cover Plate of the Vacuum Manifold" on page 92.

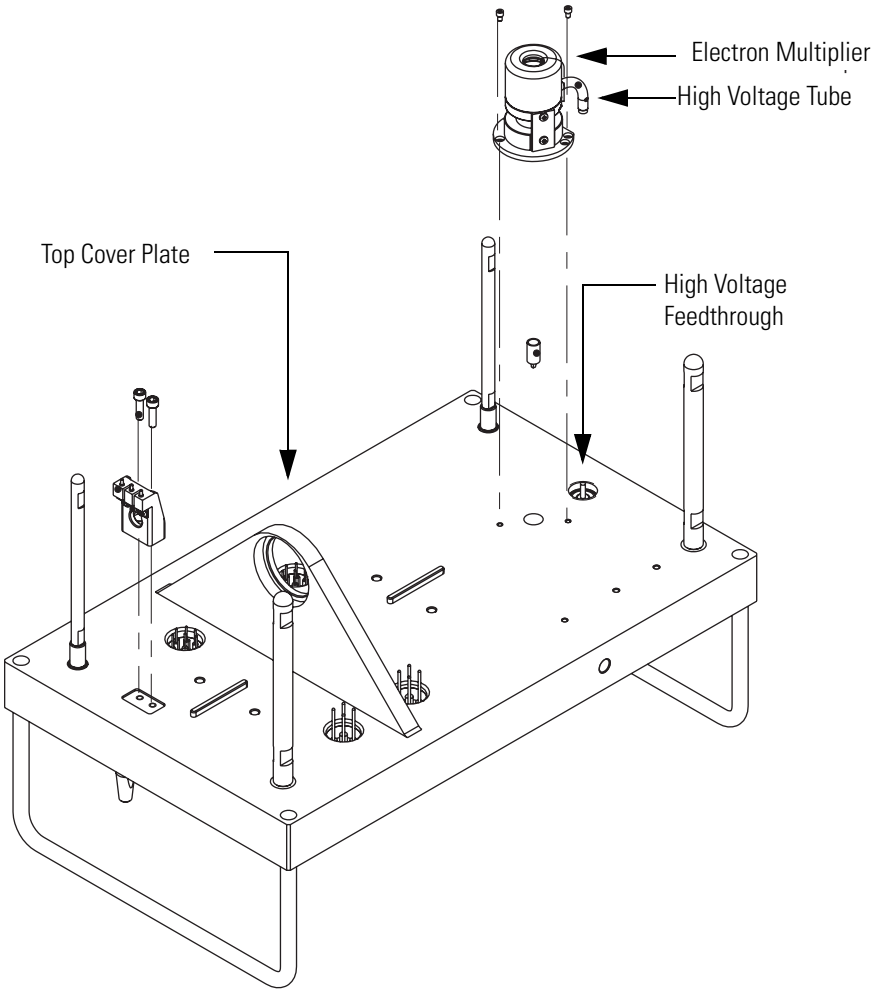
IMPORTANT Wear clean, lint-free, nylon or cotton gloves when you handle the electron multiplier components.

4. With an Allen wrench and wearing clean, lint-free, nylon or cotton gloves, remove the two socket-head screws that hold the electron multiplier support to the top cover plate of the vacuum manifold. See Figure 45.
5. With one hand holding the high voltage tube and with the other hand holding the electron multiplier support, 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.)

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

6. 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 as shown in Figure 45.

Figure 45. Installing the electron multiplier



7. Reinstall the two socket-head screws that secure the electron multiplier support to the top cover plate. Tighten the screws with an Allen wrench.
8. Reinstall the top cover plate of the vacuum manifold over the opening in the vacuum manifold as described in "Reinstalling the Top Cover Plate of the Vacuum Manifold" on page 100.
9. Reinstall the top cover of the MS detector as described in "Reinstalling the Top Cover of the MS Detector" on page 100.
10. After you replace the electron multiplier, calibrate it as described in the next section.

Calibrating the Electron Multiplier

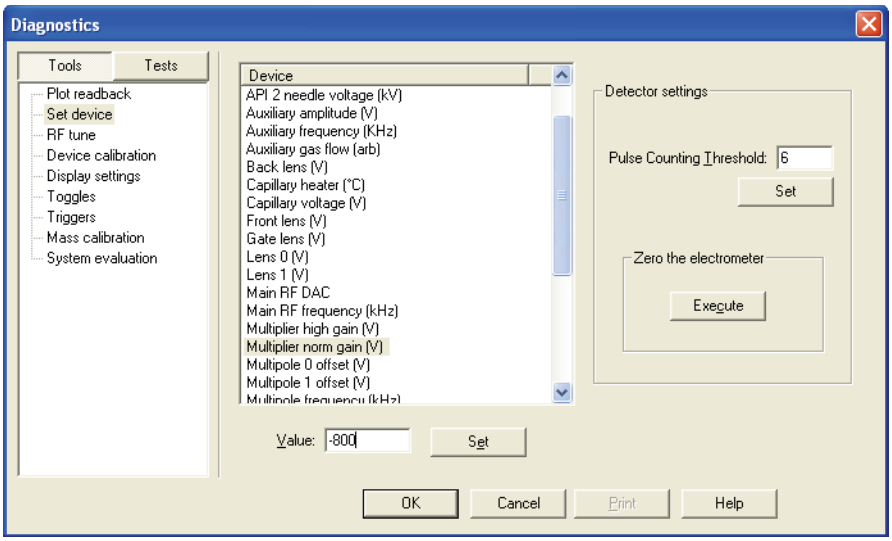
Calibrate the electron multiplier after you replace it.

❖ To calibrate the electron multiplier

1. Start up the LCQ Fleet system as described in "Starting the System after a Complete Shutdown" on page 115.
2. Set the electron multiplier voltage to -800 V as follows:
   a. Make sure that the system is in the MS/MS mode.
   b. From the Windows XP taskbar, choose **Start > All Programs > Xcalibur > LCQ Fleet Tune** to open the Tune Plus window.
   c. From the Tune Plus window, choose **Diagnostics > Diagnostics**.

   The Diagnostics dialog box appears. See Figure 46.

   Figure 46. Diagnostics dialog box



   d. Under **Tools**, select **Set device**.
   e. Under **Device**, select **Multiplier norm gain**.
   f. In the **Value** box, type **-800**.
   g. Click **Set** to set the electron multiplier voltage to -800 V.
   h. Click **OK** to return to Tune Plus.
3. To calibrate the electron multiplier voltage
   a. Pump down the system for at least one hour before you turn on the high voltages.
   b. Set up to infuse tuning solution into the MS detector as described in the *LCQ Fleet Getting Started Guide*.

c. From the Tune Plus window, choose **Control > Calibrate**.

   The Calibrate dialog box appears.

d. Choose **View > Display Graph View**.

e. Click the **Semi-Automatic** tab to display the Semi-Automatic page.

f. Under **What to Calibrate**, select **Electron Multiplier Gain**.

g. To start the multiplier gain procedure, click **Start**.

4. After the Electron Multiplier Gain program is finished, set up for operation as described in the *LCQ Fleet Getting Started Guide*.

Replacing the Turbomolecular Pump Cartridge

Plan to replace the rotating, interior portion of the turbomolecular pump, referred to as the turbomolecular pump cartridge, after 20000 to 30000 hours of operation, or if the bearings fail.

CAUTION The turbomolecular pump insert is very delicate. We recommend that a Thermo Scientific field service engineer replace the turbomolecular pump insert.

❖ To replace the turbomolecular pump cartridge

1. Shut down the system.
2. Remove the left front panel.
3. Disconnect the power cable from the turbomolecular pump.
4. Disconnect the foreline from the turbomolecular pump.
5. Loosen and remove the six 4-mm socket-head screws that hold the insert to the pump.
6. Remove the old cartridge and install a new cartridge.
7. Install and tighten the six screws that hold the cartridge to the pump.
8. Connect the foreline to the turbomolecular pump.
9. Connect the power cable to the turbomolecular pump.
10. Reinstall the left front panel.
11. Start the system.

Cleaning the Fan Filter

You must clean the fan filter (P/N 97055-20254) every four months. The fan filter is located on the back of the MS detector on the right side (when viewed from the front).

❖ To clean the fan filter

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

System Shutdown, Startup, and Reset

If you will not be using the system for 12 hours or more, you can place the LCQ Fleet system in Standby mode to conserve nitrogen. To perform maintenance procedures on system components that are held under vacuum, you must shut down the MS detector completely.

This chapter contains the following sections:

Shutting Down the System in an Emergency

In emergency situations, you can turn off the MS detector and the vacuum pumps.

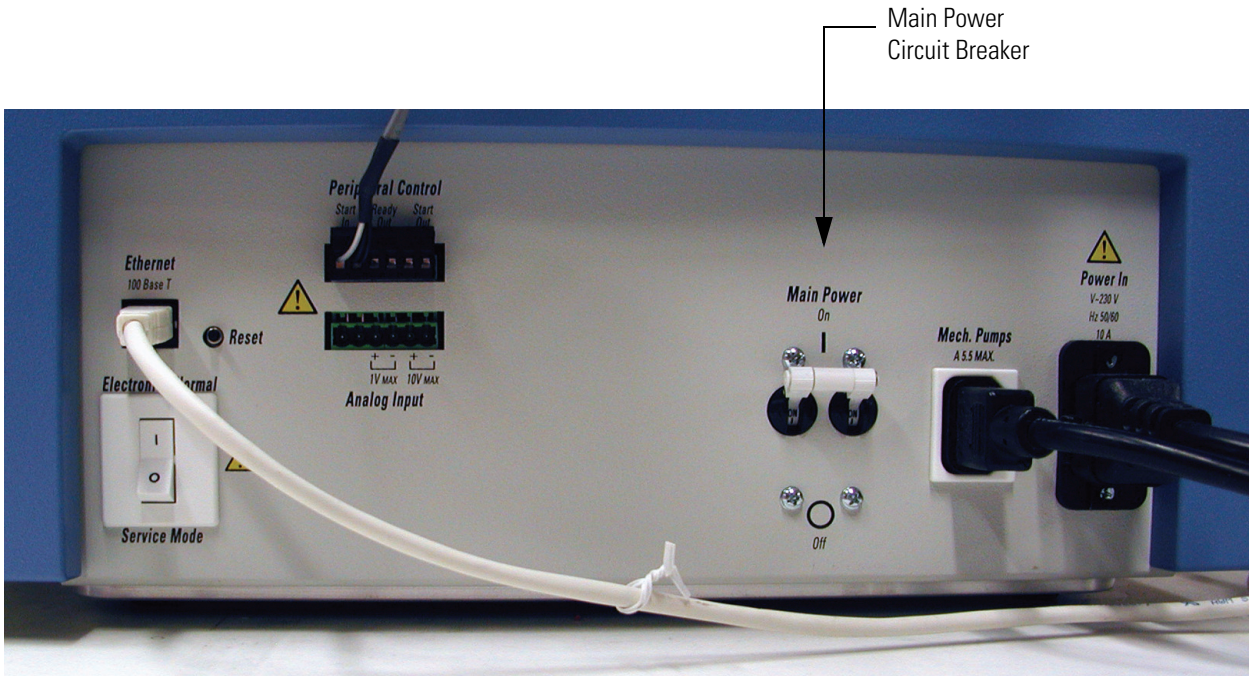
❖ **To perform an emergency shutdown of the LC/MS system**

1. 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 47), 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, Thermo Scientific does not recommend doing so. Instead, follow the procedure "Shutting Down the System Completely" on page 113.

2. To turn off the LC pump, autosampler, and computer in an emergency, use the on/off switches for these devices.

Figure 47. View of the power panel showing the Reset button and the main power circuit breaker



Placing the System in Standby Mode

You do not need to shut down the LCQ Fleet 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 Standby mode.

❖ **To place the LCQ Fleet MS detector in Standby mode**

1. Wait until data acquisition, if any, is complete.
2. To turn off the solvent flow from the LC pump

   a. In the Tune Plus window, click 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 mode. 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 the **On/Standby button** to toggle it to Standby). The MS detector in now in Standby mode.

When you put the MS detector in Standby, the LCQ Fleet turns off the electron multiplier, conversion dynode, 8 kV power to the API source, main RF voltage, and ion guide RF voltages. The LCQ Fleet also turns off the auxiliary and sheath gas flows. See Table 10 on page 120 for the On/Off status of MS detector components when the MS detector is in Standby mode. The System LED on the front panel of the MS detector is yellow when the system is in Standby.

4. Flush the spray cone and the entrance end of the ion transfer capillary of the API source as described in "Flushing the Ion Sweep Cone and Ion Transfer Capillary" on page 72.
5. Purge the forepump oil as described in "Purging the Oil in the Forepump" on page 66.
6. Leave the power on for the following components of your LC/MS system:
   - The MS detector
   - The LC pump
   - The autosampler
   - The data system computer

Shutting Down the System Completely

If you are not going to use LCQ Fleet MS detector for a short period of time, such as overnight or over weekends, you do not need to shut it down completely (see "Placing the System in Standby Mode" on page 112). Shut down the system completely only if you do not plan to use it for an extended period or if it must be shut down for a maintenance or service procedure.

❖ To shut down the LCQ Fleet completely

1. Turn off the solvent flow from the LC pump (or other sample introduction device).

   Note For instructions on how to turn off the solvent flow from the LC pump, refer to the Help provided with the software.

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

   When you place the MS detector in Standby, the LCQ Fleet turns off the electron multiplier, conversion dynode, 8 kV power to the API source, main RF voltage, and octapole RF voltage. In addition the LCQ Fleet turns off the flow of the sheath and auxiliary gasses.

3. Place the electronics service switch, located on the power panel (see Figure 47 on page 112), in the Service position.

Placing the electronics service switch in the Service position turns off the power to the non-vacuum system electronics.

4. Place the main power circuit breaker switch in the Off (O) position.

   The switch is located on the power panel (Figure 47). When this switch is turned off, the following occurs:

   - All power to the MS detector, including the turbomolecular pump and forepump, is turned off. (All LEDs on the front panel of the MS detector are off.)
   - 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 5 minutes, 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 pump, 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, Thermo Scientific recommends that you turn off the LC pump, data system computer, and autosampler as described in steps 6 through 11.

6. Turn off the LC pump (if it is a part of your system). 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. In the Windows XP® Start menu, click the **Shutdown** button.

      The Shut Down Windows dialog box appears.

   b. Select **Shut Down**, and then click **OK** to start the Windows XP shutdown procedure.

   c. 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 printer (if it is a part of your system) by using the printer on/off switch.
11. Turn off the autosampler (if it is a part of your system) by using the autosampler main power on/off switch.

Starting the System after a Complete Shutdown

To start up the LCQ Fleet after it has been shut down completely, you must perform the following steps:

1. Starting the LC Pump (if this is a part of the system)
2. Starting the Data System
3. Starting the MS Detector
4. Starting the Autosampler (if this is a part of the system)
5. Setting Up Conditions for Operation

Starting the LC Pump

To start the LC pump, follow the startup procedure described in the manual that came with the LC pump. If necessary, configure the LC pump as described in the manual provided with the LC Devices software. Do not turn on the solvent flow to the MS detector.

Starting the Data System

❖ **To start the data system**

1. Turn on the monitor, computer, and printer.
2. Follow the Windows XP startup procedure.
3. Press **CTRL + ALT + DEL** when you are prompted to do so, and then click **OK** or enter your password (if you have one) in the Logon Information dialog box to complete the startup procedure.

Starting the MS Detector

❖ **To start the MS detector**

Note The data system must be running before you start 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 forepump and the turbomolecular pump start. All LEDs on the MS detector front panel are off.
5. Allow the LCQ Fleet to pump down for 5 minutes.
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 turns 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 turns 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 turns 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 three minutes, the System LED turns 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 turns green only if the pressure in the vacuum manifold is below the maximum allowable pressure (5×10^{-4} Torr in the analyzer region, and 2 Torr in the capillary-skimmer region).

If you have an autosampler, see "Starting the Autosampler" on page 116. If you do not have an autosampler, go to the topic "Setting Up Conditions for Operation" on page 117.

Starting the Autosampler

To start 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, and so on, refer to the manual supplied with the autosampler. You can find information on connecting your autosampler to the LCQ Fleet MS detector in the *LCQ Fleet Getting Connected Guide*.

Setting Up Conditions for Operation

❖ **To set up your LCQ Fleet for operation**

1. Before you begin data acquisition with your LCQ Fleet, allow the system to pump down for at least one 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 proper LCQ Fleet 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 the *LCQ Fleet Getting Started Guide*.

   Note You do not need to calibrate or tune the LCQ Fleet each time you restart it.

   Calibration parameters are instrument parameters whose values do not vary with the type of experiment, such as the ionization mode or the solvent flow rate. Calibrate the LCQ Fleet once a month. Check the calibration once a week by viewing the mass spectrum of an analyte for which you have recorded data. If the measured mass-to-charge ratios for the known analytes changes, re-calibrate the MS detector. Refer to the *LCQ Fleet Getting Started Guide* for the LCQ Fleet calibration procedure.

   Tune parameters are instrument parameters whose values vary with the type of experiment. Tune the LCQ Fleet (or change the tune method) whenever you change the type of experiment. Refer to *LCQ Fleet Getting Started Guide* for tuning procedures in the ESI or APCI mode. The LCQ Fleet comes with several standard tune methods that are specific for various experimental conditions.

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. Pressing the Reset button creates an interruption in the embedded computer that causes it to restart in a known (default) state. See Figure 47 on page 112 for the location of the Reset button.

Note The Reset button is a momentary switch. After you release it, it returns to its normal position.

This procedure 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, see "Starting the System after a Complete Shutdown" on page 115.

❖ **To reset the MS detector**

Press the Reset button located on the power panel, and then verify that the Communication LED is extinguished.

When you press the Reset button, the following occurs:

- An interruption of 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 turns 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 turns 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 three minutes the software transfer is complete. The System LED turns either green or yellow. Green indicates that the instrument is functional and the high voltages are on. Yellow indicates that the instrument is functional and is in Standby mode.

Resetting the Tune and Calibration Parameters to their Default Values

You can reset the LCQ Fleet tune and calibration parameters to their default values at any time. This feature might be useful if you have manually set some parameters that have resulted in less than optimal performance.

❖ **To reset the LCQ Fleet tune and calibration parameters to their default values**

Note Make sure that the problems that you are experiencing are not due to improper API source settings (for example, spray voltage, sheath and auxiliary gas flow, ion transfer capillary temperature, and so on) 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 LCQ Fleet system parameters (that is, to calibrate or tune the system), perform the calibration procedure described in the *LCQ Fleet Getting Started Guide*.

Resetting the Data System

There are two ways to reset the data system:

- Using Windows XP to Reset the Data System
- Using the Reset Button on the PC to Reset the Data System

Using Windows XP to Reset the Data System

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 Windows XP

1. From the Windows XP task bar, choose **Start > Turn Off Computer**.

   The Turn Off Computer dialog box appears.

2. Click the Restart button to start the Windows XP shutdown and restart procedure.

3. Press **CTRL + ALT + DEL** when prompted, and then click **OK** or enter your password (if you have one) in the Logon Information dialog box to complete the shutdown and restart procedure.

Note Resetting the data system automatically re-establishes the communications link between the data system and the MS detector. When this link occurs, the Communication LED on the front panel of the MS detector turns yellow and then green. If the system is unable to re-establish the communications link, press the Reset button on the power panel of the MS detector. Press the Reset button quickly and firmly.

Using the Reset Button on the PC to Reset the Data System

❖ To reset the data system by pressing the reset button on the computer

1. Press the reset button on the personal computer.

2. Observe the Windows XP shutdown and restart procedure on the monitor, and press **CTRL + ALT + DEL** when prompted. To complete the shutdown and restart procedure, click **OK** or enter your password (if you have one) in the Logon Information dialog box.

3. When the shutdown and restart procedure is complete, choose **Start > All Programs > Xcalibur > LCQ Fleet Tune**.

   The Tune Plus window appears.

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 turns yellow and then green. If the system is unable to reestablish the communications link, press the Reset button on the power panel of the MS detector. Only a momentary push of the Reset button is needed as it is a momentary switch.

Turning Off Selected MS Detector Components

You can turn off some or all of the MS detector components five ways:

- 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 in which to leave the MS detector when it is not in use. Choose **Control > Standby** (or click the On/Standby button) from the Tune Plus window.
- Turn the MS detector off. Off 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 mode.
- Turn the electronics service switch to Service. The electronics service switch allows you to perform maintenance procedures involving system components of the MS detector that are not under vacuum.
- 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 10.

Table 10. On/off status of MS detector components, voltages, and gas flows (Sheet 1 of 2)

MS detector component	Standby mode 	Off mode 	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

Table 10. On/off status of MS detector components, voltages, and gas flows (Sheet 2 of 2)

MS detector component	Standby mode 	Off mode 	Electronics service switch in Service position	Main power circuit breaker switch in Off (O) position
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	On	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
Turbomolecular pump	On	On	On	Off
Rotary-vane pump	On	On	On	Off
Turbomolecular Pump Controller	On	On	On	Off
Power supply, electron multiplier/conversion dynode	Off	Off	Off	Off
Power supply, 8 kV	Off	Off	Off	Off
Power supply PS1	On	On	Off	Off
Power supply PS2	On	On	On	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

Diagnostics and PCB and Assembly Replacement

Many of the MS detector components can be tested by the LCQ Fleet diagnostics. Thermo Scientific's service philosophy for the LCQ Fleet system calls for troubleshooting to the lowest part, assembly, PCB, or module listed in Chapter 7, "Replaceable Parts." Plan to replace LCQ Fleet components when indicated by the LCQ Fleet diagnostics, by Thermo Scientific Technical Support, or by a Thermo Scientific Customer Support Engineer.

This chapter contains the following sections:

Running the LCQ Fleet Diagnostics

The LCQ Fleet diagnostics 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 LCQ Fleet diagnostics can often locate the problem. You can often correct the problem yourself by replacing a faulty PCB or assembly.

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

Before running the diagnostics, 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. Check that alignment, configurations, and cable connections are correct before you run the LCQ Fleet diagnostics.

To run the LCQ Fleet diagnostics, perform the following steps:

1. Calibrating the Multipole RF and the Main RF
2. Running the Diagnostics

Calibrating the Multipole RF and the Main RF

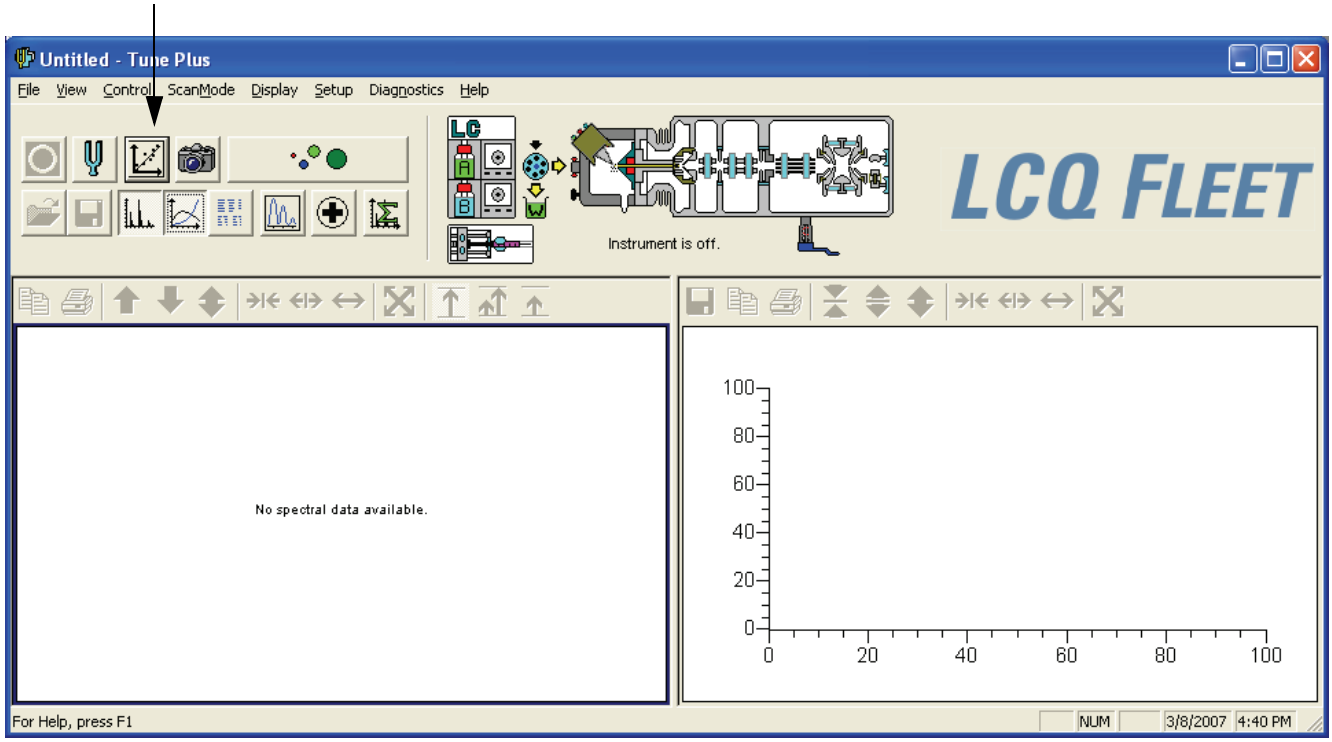
Proper calibration of the multipole RF frequency is necessary to allow for the maximum transmission of ions through the multipoles. You need to calibrate the frequency of the multipole RF voltage each time you modify the hardware in some way, for example, by a maintenance operation.

❖ To calibrate the multipole RF and the main RF

1. Click **Calibrate** in the Tune Plus window task bar (Figure 48). You can also access Calibrate from the Control menu at the top of the Tune Plus window by choosing **Control > Calibrate**.

   The Calibrate dialog box appears. See Figure 49.

Figure 48. LCQ Fleet Tune Plus window



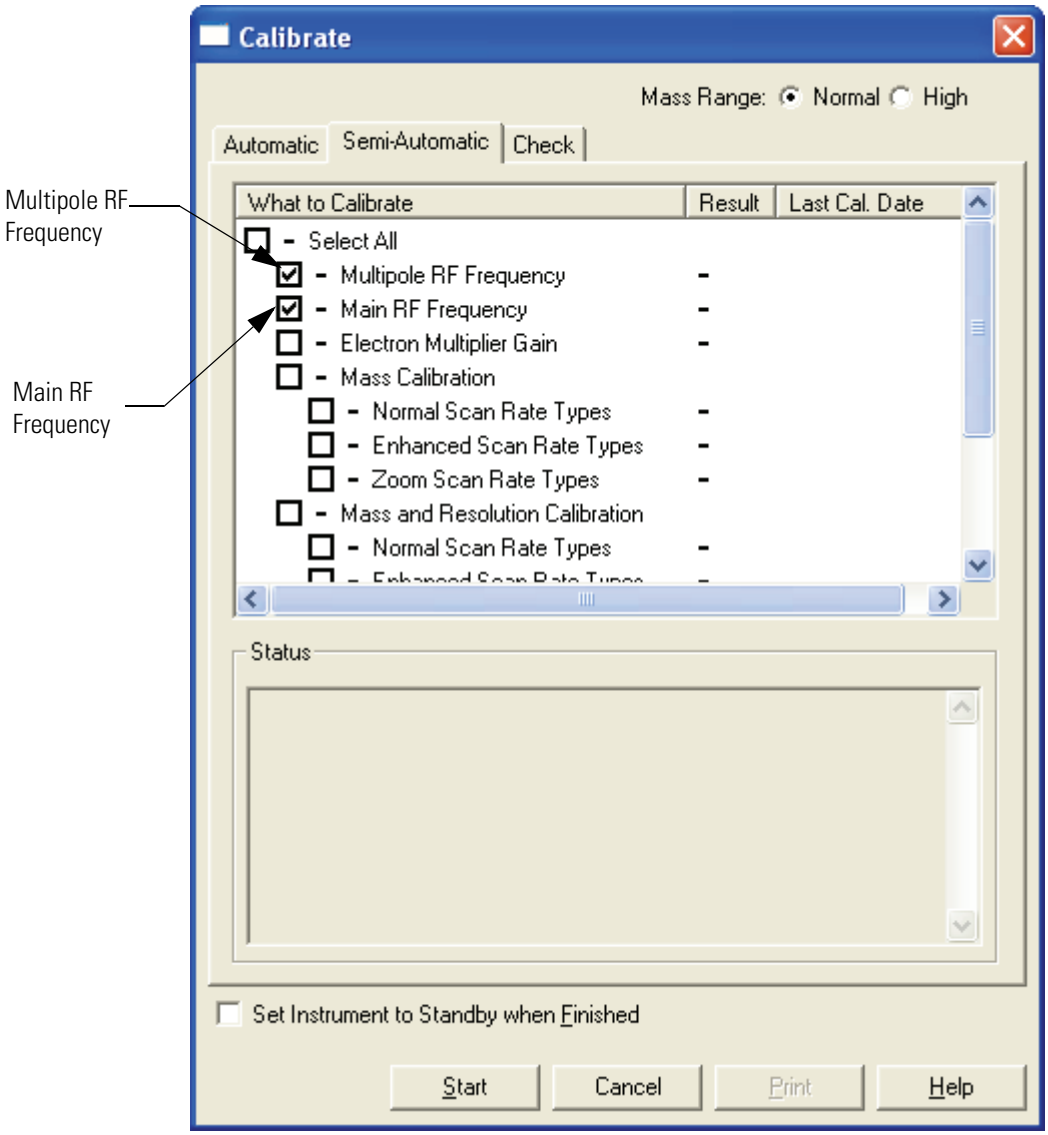
2. Click the **Semi-Automatic** tab.

   Figure 49 shows the Semi-Automatic page of the Calibrate dialog box.

3. In the **What to Calibrate** area, select the **Multipole RF Frequency** and **Main RF Frequency** check boxes.

4. Click **Start**.

Figure 49. Calibrate dialog box. Multipole RF Frequency and Main RF Frequency are indicated.



After you click the Start button (see Step 2 above), the instrument carries out an automated sequence of steps that the data system displays as graphs in the Graph view of the Tune Plus window. The titles of the graphs are as follows:

- Coarse Tune - multipole resonance frequency (Figure 50)
- Scanning Multipole RF DAC graph (Figure 51)
- Tuning RF Resonance Frequency (Figure 52)

The graphs shown in Figure 51 through Figure 52 appear automatically as the instrument goes through the tuning procedure.

Figure 50. Coarse Tune - multipole resonance frequency

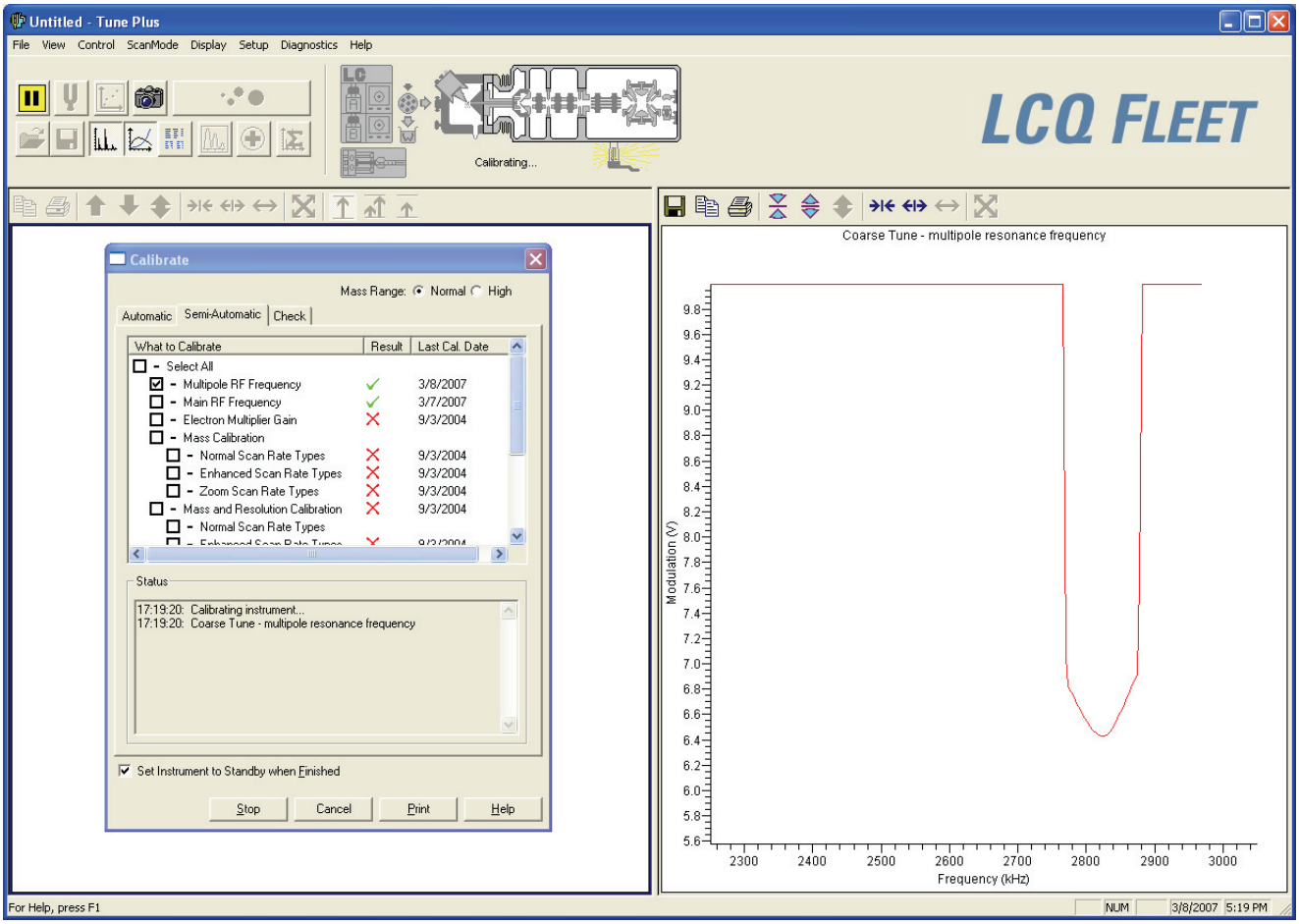


Figure 51. Scanning Multipole RF DAC graph

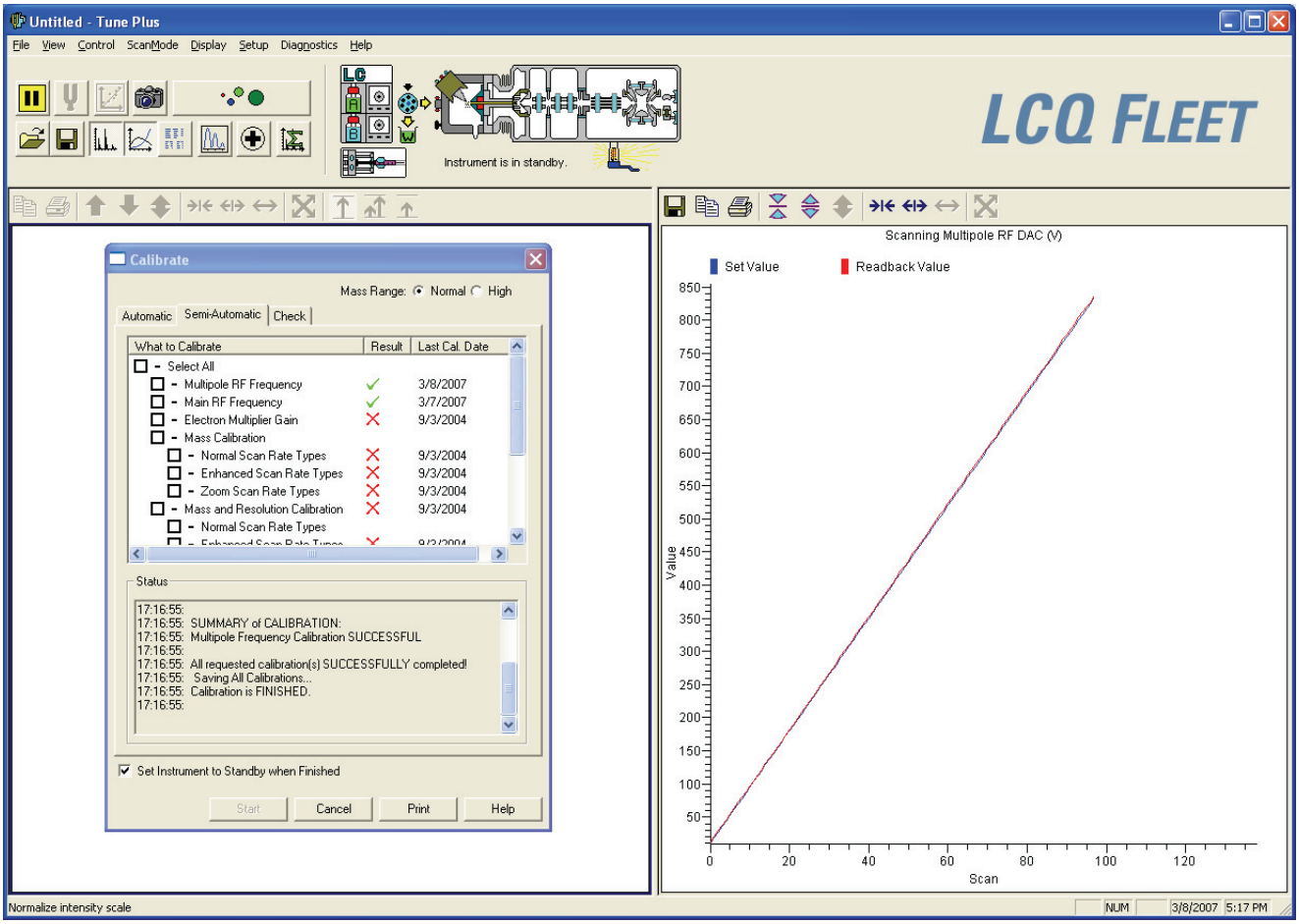
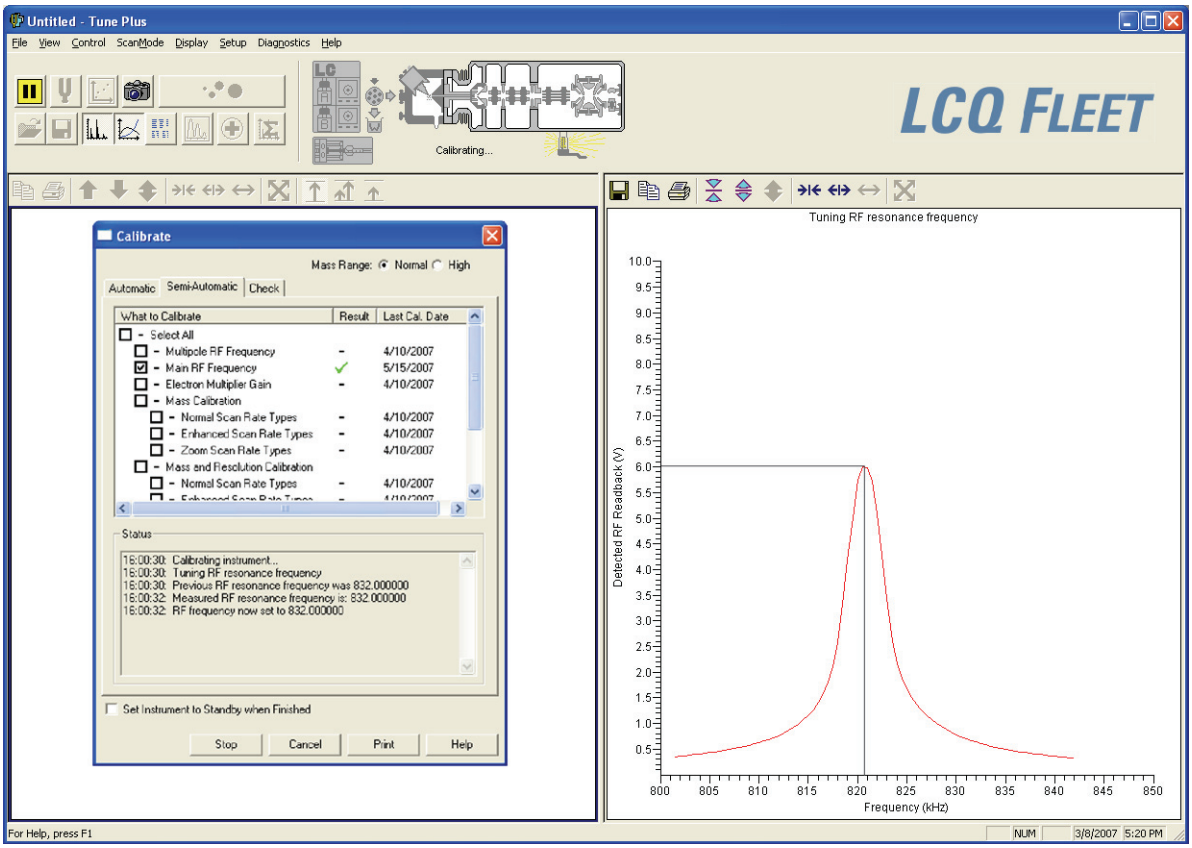


Figure 52. Tuning RF resonance frequency



Running the Diagnostics

❖ To run the diagnostics

1. In the LCQ Fleet Tune window, choose **Diagnostics > Diagnostics**.

   The Diagnostics dialog box appears (Figure 53).

2. Click the **Test** tab (Figure 53).

3. Depending on what you want to test, do one of the following:

   - To perform testing on all the subsystems (except for the I/O test that requires a special test fixture), go to step 4.
   - To perform testing on specific subsystems, go to step 5.

4. To select all the subsystems, do the following:

   a. Under **General**, select **All**.

   b. Under **What to Test**, select the **All tests** check box.

The check boxes of the subsystems under ALL TESTS are automatically selected, which ensures that all of the electronic subsystems (that is, power supplies, lenses, ion detection system, electronics and RF system) will undergo testing. See Figure 53.

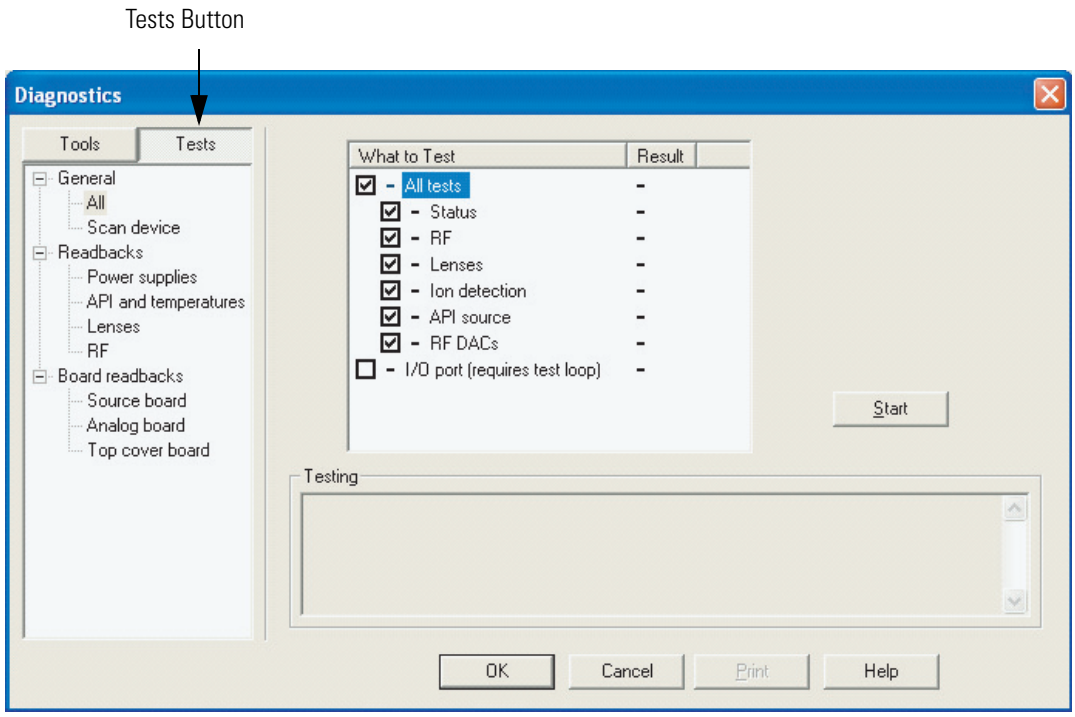
c. Go to step step 6.

5. To test an individual subsystem, select the check box corresponding to that subsystem in the What to Test area.

6. Click **Start** to start the diagnostics.

The LCQ Fleet starts testing and displays a chronological log of all diagnostic tests in the Testing box. Once testing for a specific subsystem is complete, the LCQ Fleet displays either a Pass (green check mark) or a Fail (red X) in the Result group box. If the LCQ Fleet diagnostics indicate a problem, follow the maintenance procedure as instructed by one of the following: a) the LCQ Fleet diagnostics, b) Thermo Scientific Technical Support, c) a Thermo Scientific Customer Support Engineer. For more information on the LCQ Fleet diagnostics, refer to the LCQ Fleet online Help.

Figure 53. Diagnostics dialog box showing All Tests checked.



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 11.

Check fuses when power is lost to a fused subsystem.

CAUTION Before you replace fuses, always shut down the system and disconnect the power cord

Use only the fuses specified in Table 11. Never replace a fuse with a fuse of a different type, voltage, or current rating.

Table 11. MS detector fuses

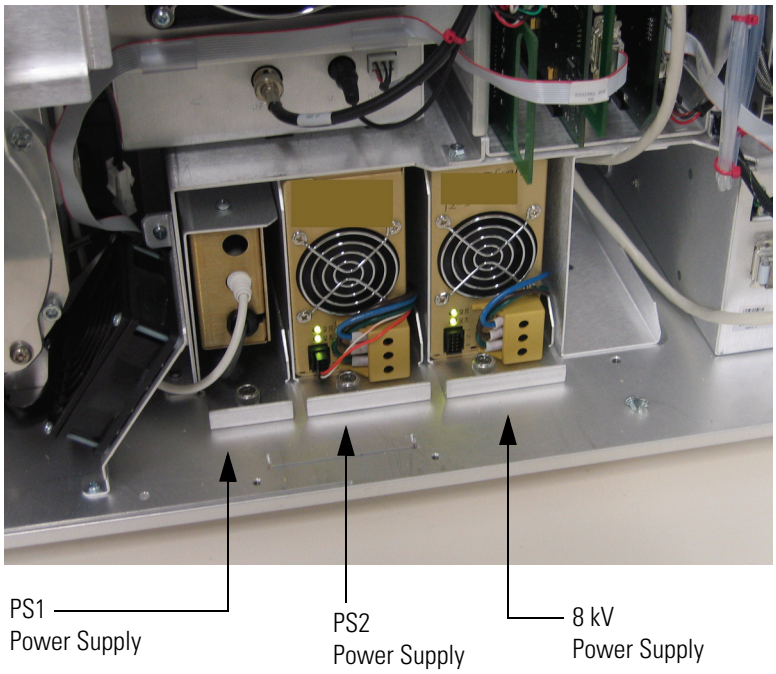
Location	Fuse	Circuit	Description	Part Number
Interlock PCB	F1,F3	APCI vaporizer heater	3.15 A, Type F, 5 × 20 mm, 250 V	00006-10510
Interlock PCB	F2, F4	220 Vac	6.3 A, 250 V	00006-11450
Source PCB	F3		4.0 A, 250 V	00006-11420

Replacing Power Supplies

The LCQ Fleet uses the following power supplies. They are easily accessed from the front of the LCQ Fleet if service or replacement is needed. See Figure 54.

- PS1 power supply (P/N 97055-60014S)
- PS2 power supply (P/N 97055-60015S)
- 8 kV power supply (P/N 97355-60003)

Figure 54. Power supplies



❖ To replace the power supplies

1. Shut down and vent the system as described in "Shutting Down the System Completely" on page 113.

CAUTION Make sure to unplug the LCQ Fleet power cord before you proceed.

2. Open the right front door of the MS detector by loosening the Allen screw on the right door.
3. If necessary, remove the left front cover as follows:
   a. If necessary, remove the Ion Max ion source housing as described in "Removing the Ion Max Ion Source Housing" on page 77.
   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. 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.

The power supplies in the Power Supply Housing have bulkhead connectors on the back.

6. Unpack the new power supply. Retain the packing materials so that you can pack and ship the defective switching power supply assembly to theThermo Scientific 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 that the old power supply once occupied. Push carefully on the power supply to seat the connectors in the back.
8. Tighten 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 "Reinstalling the Ion Max Ion Source Housing" on page 85.
11. Close the right front door of the MS detector. Tighten the Allen screw on the right front door.
12. Restart the system as described in "Starting the System after a Complete Shutdown" on page 115.
13. Run the LCQ Fleet diagnostics to verify that the system is operational.

Replacing PCBs in the MS Detector

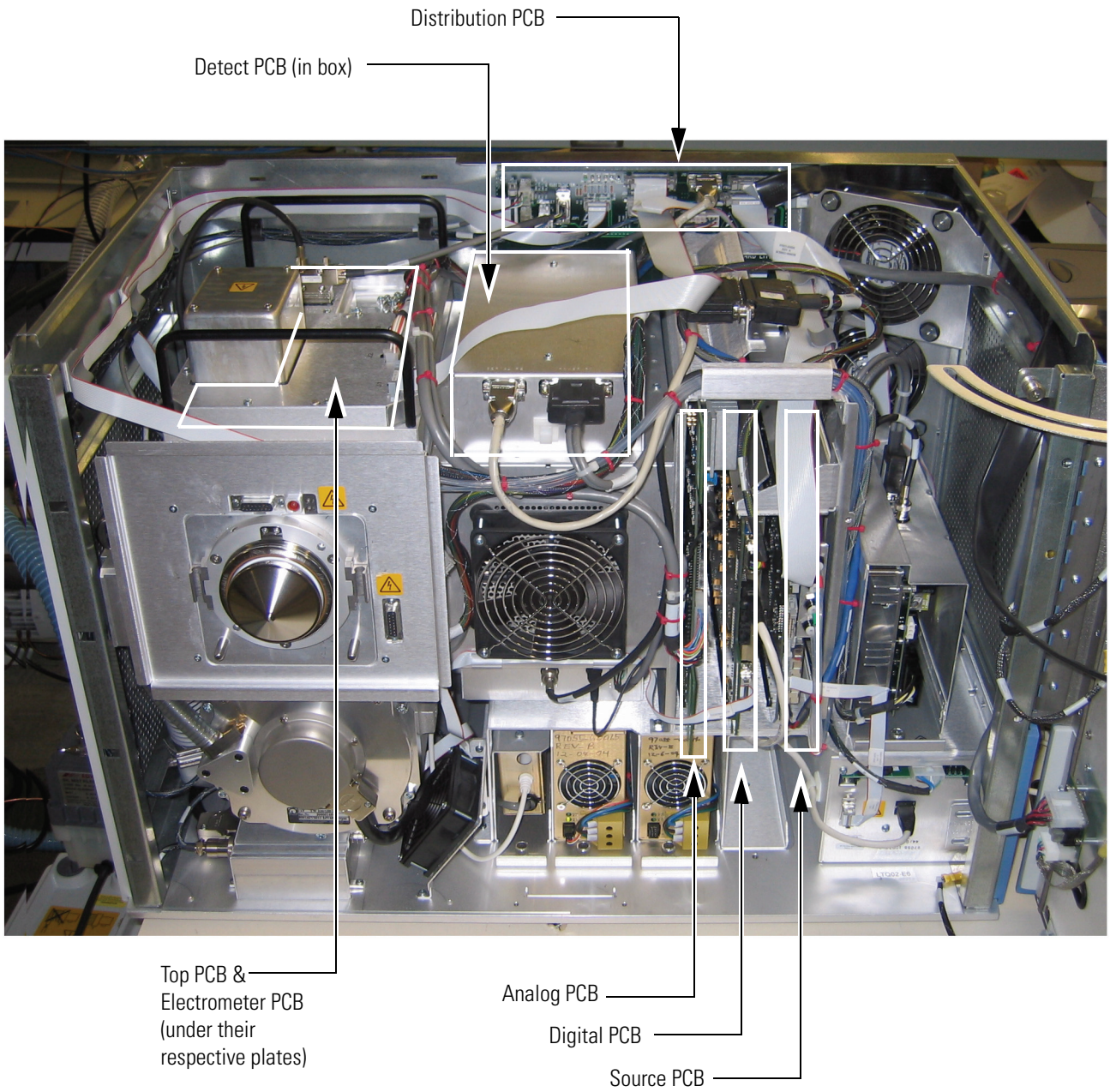
The LCQ Fleet electronic assemblies are close-packed to minimize the size of the system. Because of the complexity of removing and reinstalling many of the LCQ Fleet PCBs, we recommend that a Thermo Scientific Field Service Engineer replace and reinstall the electronic assemblies.

Figure 55 shows the PCBs in the MS detector.

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

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

Figure 55. MS detector PCBs



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 LCQ Fleet system, order only the parts listed or their equivalent.

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

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 the *EX* in front of the part number. for example, EX00108-01-00004.

This chapter contains the following sections:

MS Detector

Replaceable parts are available for the following:

- ESI Source
- APCI Source
- Ion Source Interface
- Q00 RF Lens
- Q0 and Q1 Ion Guides
- Mass Analyzer
- Electron Multiplier
- Coil Module
- Divert/Inject Valve
- Syringe Pump
- Turbomolecular Pump
- Forepump
- Pressure Gauges
- Vacuum Accessories
- Vacuum Manifold O-Rings
- Vent Valve
- Power Supplies
- Printed Circuit Boards (PCBs)
- 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. Figure 56 shows an exploded view of the ESI probe.

ESI Probe OPTON-20011
- Body-probe manifold, ... 97055-20300
- Nozzle-ESI probe 3-port, ... 97055-20146
- Fitting, union, ZDV, 1/4-28, PEEK, black, ... 00109-00304
- 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-in.L, 0.24-in. OD washer, ... 00950-00990
- Connector receptacle, high voltage, shielded, ... 00004-89626
- Ferrule, 0.012-in. ID (inner bore), KEL-F, HPLC, ... 00101-18116
- Fitting, Fingertight 2 Upchurch, ... 00101-18195
- Fitting, plug, 1/4-28, TEFZEL, HPLC, ... 00101-18075
- O-ring, 0.676-in. ID × 1/16 THK, Viton, ... 00107-05710
- O-ring, 0.125-in. ID × 1/16 THK, Viton, ... 00107-02550
- Assembly-resistor contact-ESI probe, ... 97055-60058
- Resistor FXD CC 1/4W 22M 5%, ROHS 00015-02-00032
- Fitting, HPLC adapter, 10-32 × 1/4-28, KEL-F, ... 00101-18080
- Tubing, fused-silica, 0.100 mm ID × 0.19 mm OD, ... 00106-10499
- Ferrule, 0.008-in. inner bore, KEL-F HPLC, ... 00101-18114

Safety Sleeve Kit. 70005-62015
- Ferrule, 0.027-in. inner bore, PEEK HPLC, ... 00101-18119
- Tube, 0.009-in. ID × 0.024-in OD, 10 inches, natural PEEK, ... 00301-22806
- Fitting, Fingertight 2 Upchurch, ... 00101-18195
- Fitting, fingertight, HPLC, 10-32, PEEK, ... 00101-18081
- Fitting, internal union for 1/16-in. OD tubing, stainless steel. 00101-18182

Figure 56. Exploded view of the ESI probe

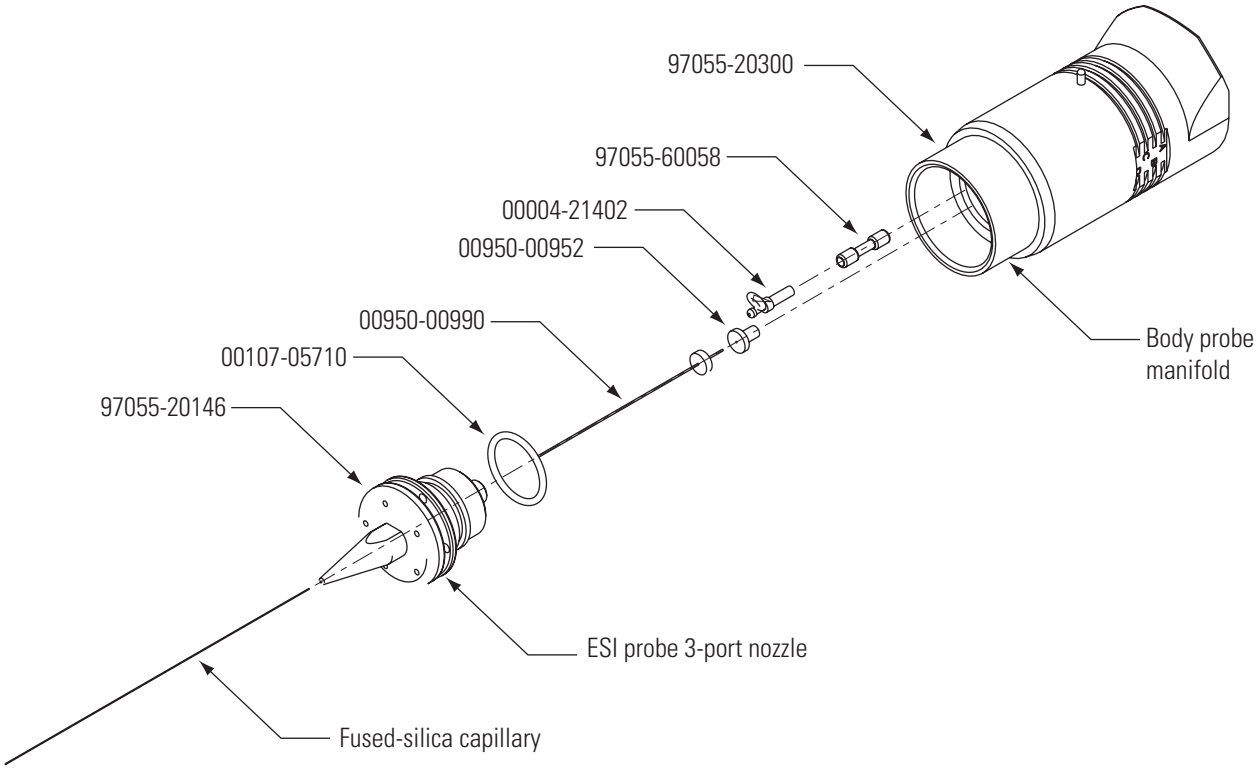
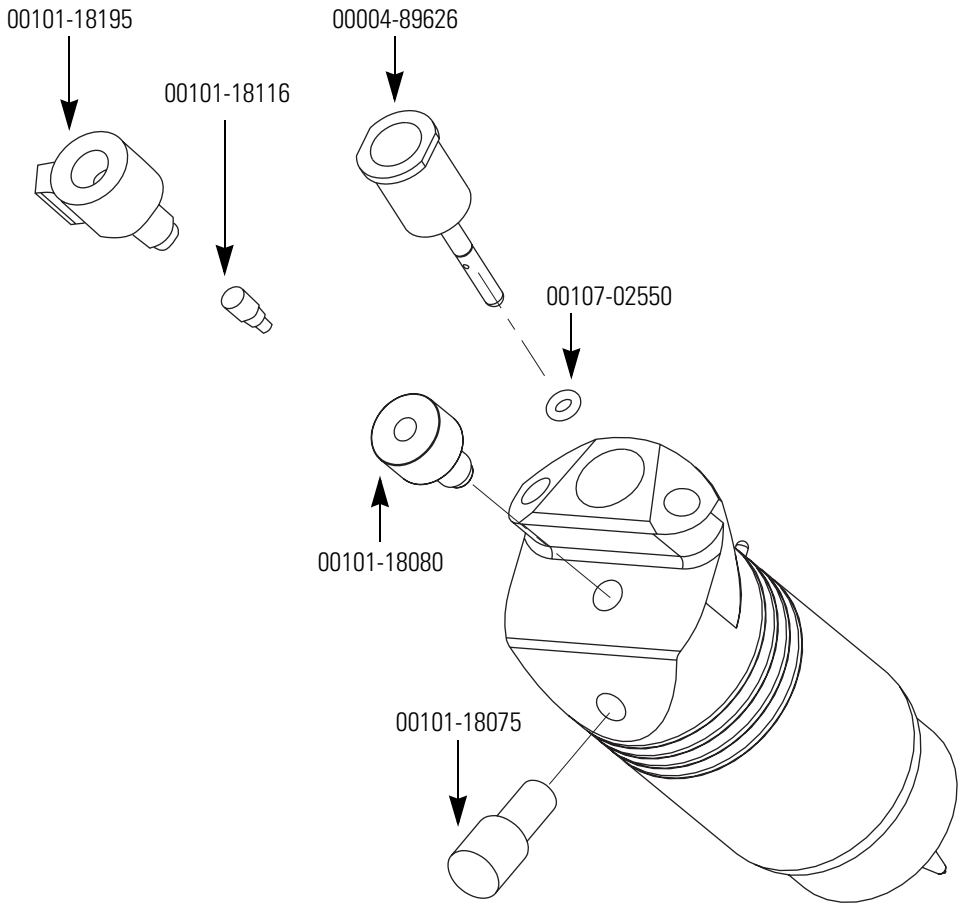


Figure 57. Replaceable parts for the ESI probe



APCI Source

Figure 58, Figure 59, Figure 60, and Figure 61 contain diagrams of the APCI probe.

APCI probe,. OPTON-20012
APCI probe nozzle assembly, ... 97055-60089
Ferrule, 0.016-in. ID, for 0.36 mm OD fused silica tubing,
PEEK HPLC,. 00101-18120
Tubing, fused silica, 0.15 mm ID × 0.363 mm OD,. 00106-10498
O-ring, 0.239-in. ID × 1/16 THK, Viton, ... 00107-04000
O-ring, 0.312-in. ID × 1/16 THK, red silicone 00107-04500
O-ring, 0.500-in. ID × 1/16 THK, Viton, ... 00107-05600
Fitting, 10-32 male nut, PEEK, ... 70005-20220
Fitting, APCI flange, ... 70005-20250
Nozzle, APCI probe,. 97055-20221
APCI probe assembly 97055-97090
Thermocouple, K-type, 1/16 × 3-in. *l*, stainless steel sheath 00007-89207
O-ring, 0.625-in. ID × 1/16-in. THK, Viton. 00107-05700
O-ring, 0.875-in. ID × 1/16-in. THK, Viton. 00107-05800
O-ring, 1.375-in. ID × 1/16-in. THK, Viton. 00107-05904
Heater, 250-300W, ceramic, 0.424-in. OD × 2.8-in. *l* 00201-99-00011
Clip, Thermocouple. 97055-20176
Tube, heater shield 97055-20233
Assembly, feedthrough, APCI probe 97055-60087
Assembly, nozzle, APCI probe-USI. 97055-60089

Figure 58. APCI probe assembly (OPTON-20012)

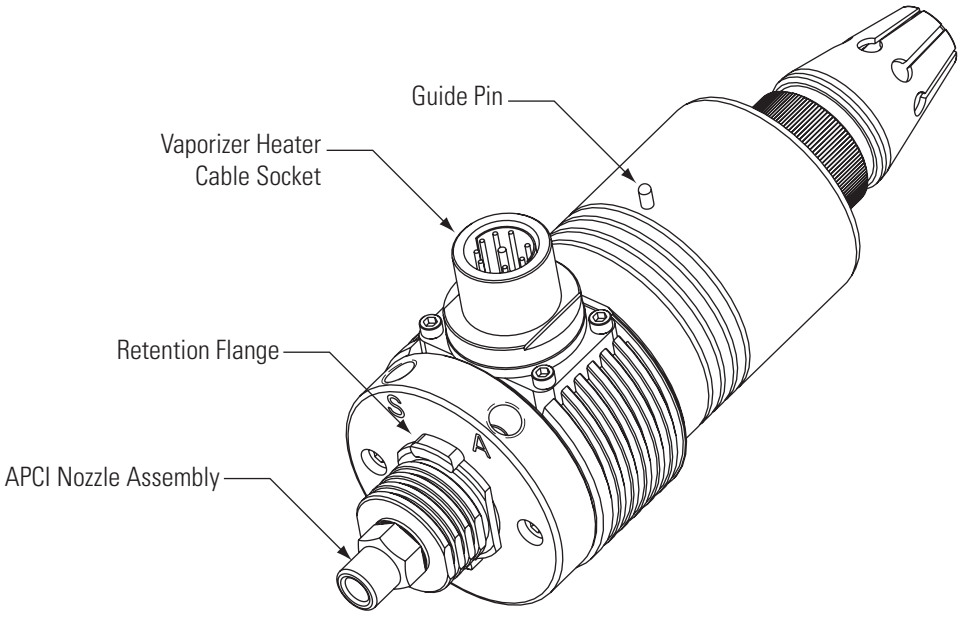


Figure 59. APCI probe nozzle assembly (P/N 97055-60089)

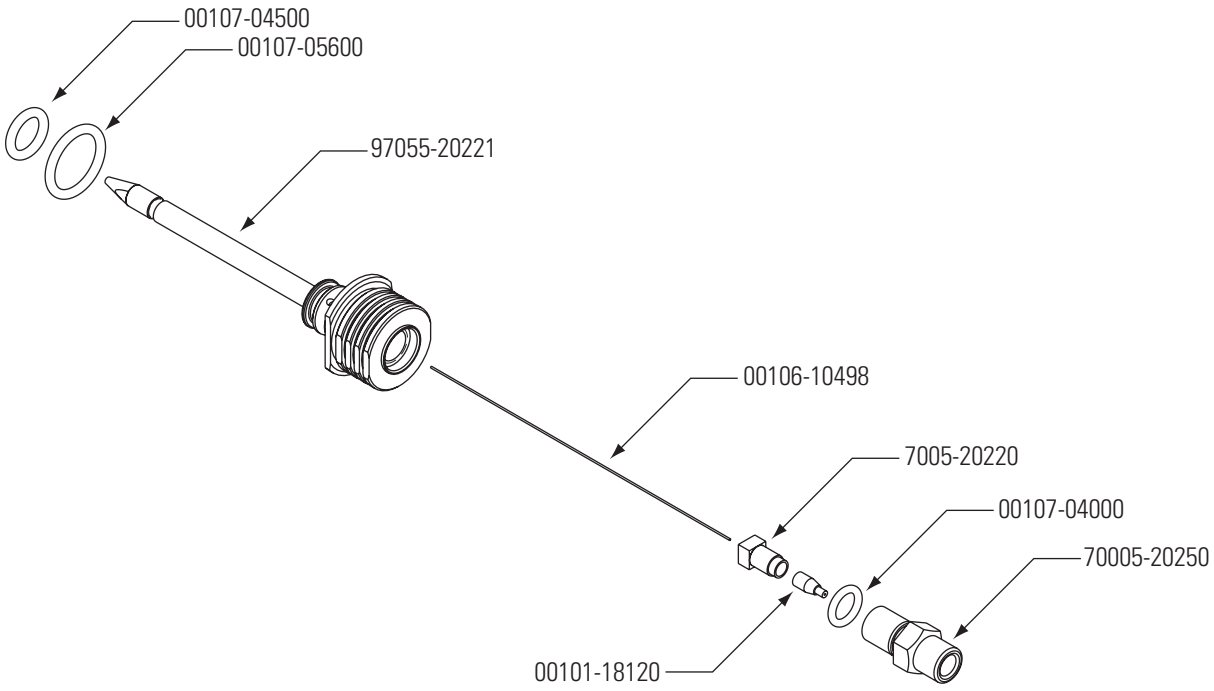


Figure 60. Assembly drawing of the APCI probe

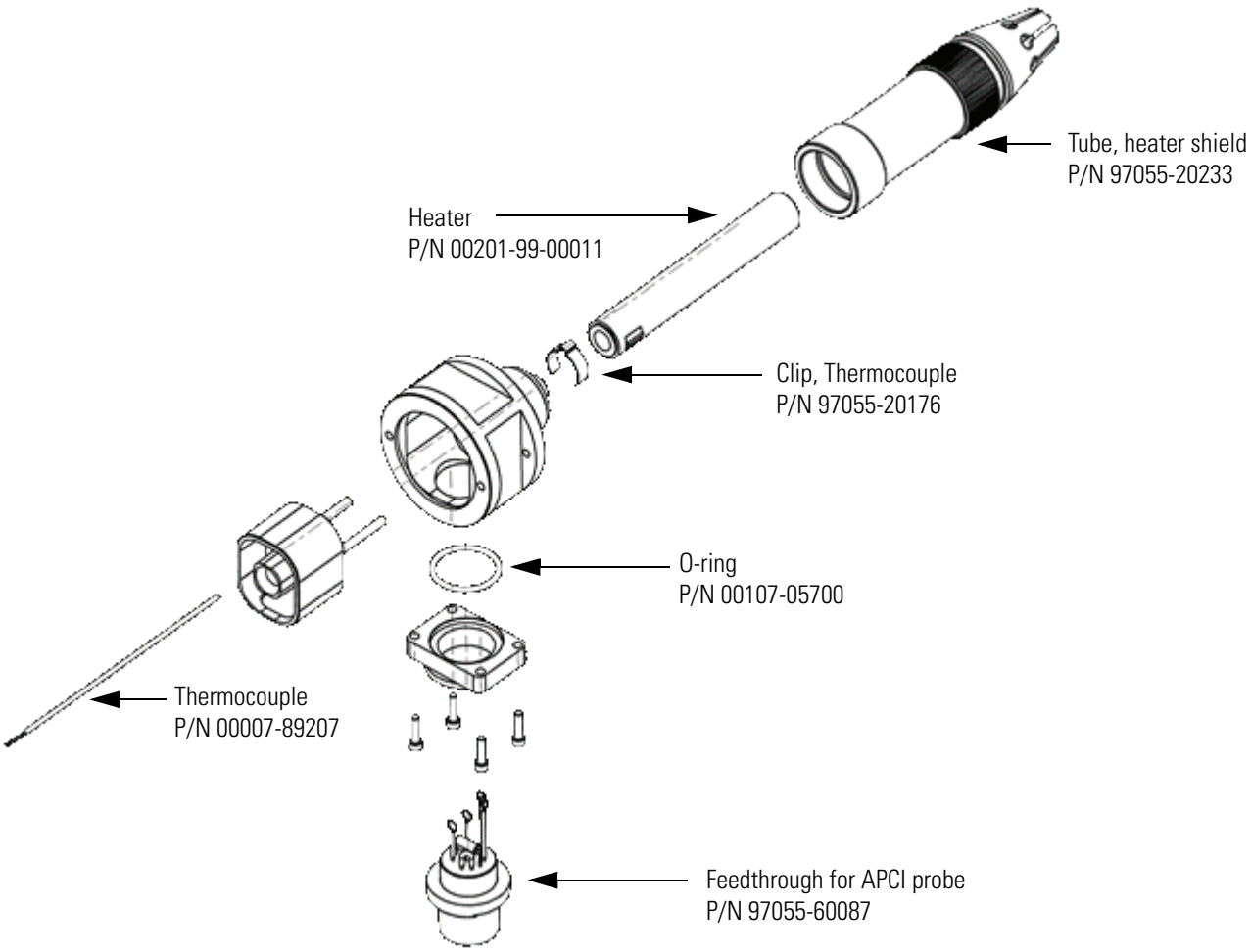
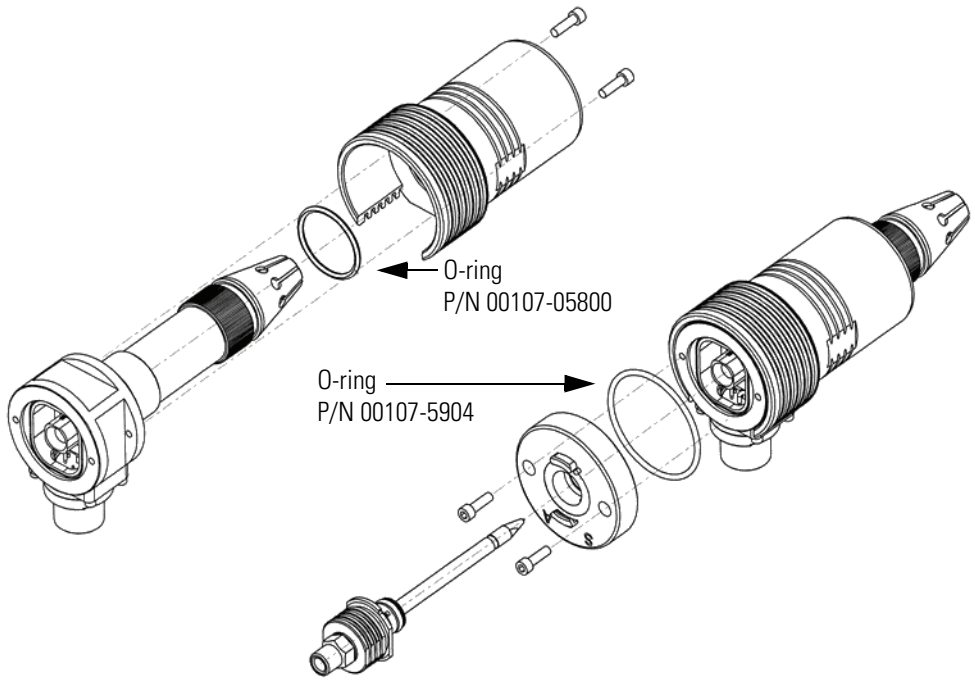


Figure 61. Assembly drawing of the APCI probe



Ion Source Interface

Ion Source Interface Assembly 97055-60181

Contact socket for 0.048 × 0.064D pin, ... 00004-89652
O-ring, 2-in. ID × 1/16 THK, 2-033 Viton V884, ... 00107-01-00006
O-ring, 2.625-in. ID × 3/32 THK, AS-146, Viton, ... 00107-11002
O-ring, 2.612-in. ID × 3/32 THK, 2-039 Viton, ... 00107-12550
O-ring, 0.325-in ID × 1/16 THK, Graphite Vespel 97055-20442
Plunger ball, 6-40 × 0.31, 1lb, ... 00201-11719
Screw, socket, 2-56 × 3/16, stainless steel, ... 00419-25603
Screw, 4-40 × 3/8-in., socket head cap, vented, stainless steel, ... 00419-44014
Screw, socket, 6-32 × 1-in., stainless steel, ... 00419-63216
Screw, set, socket, 6-32 × 7/8-in., alloy, A574, ... 00451-63278
Screw, 2-56 × 3/32, socket head, stainless steel, ... 00452-25612
Seal, graphite source heater, ... 70111-20216
Thumbnut, knurled, 6-32, UNC 97055-20033
Seal, API cone, ... 97055-20034
Cone, API source (sweep cone), ... 97055-20035
Ring, contact, support, ... 97055-20503
Capillary heater assembly, ... 97055-60176
Bushing, nose cone insulator, ... 97055-20074
Cage, capillary heater mount, ... 97055-20065
Ion transfer capillary, 500 micron, ... 97055-20517
Clamp socket, ... 97055-20203
Ion sweep cone, ... 97055-20214
Tube lens, ... 97055-20463
Skimmer, ... 97055-20516
Offset, 0.050-in, LTQ Lite 97055-20459

Figure 62. Ion source interface (front)

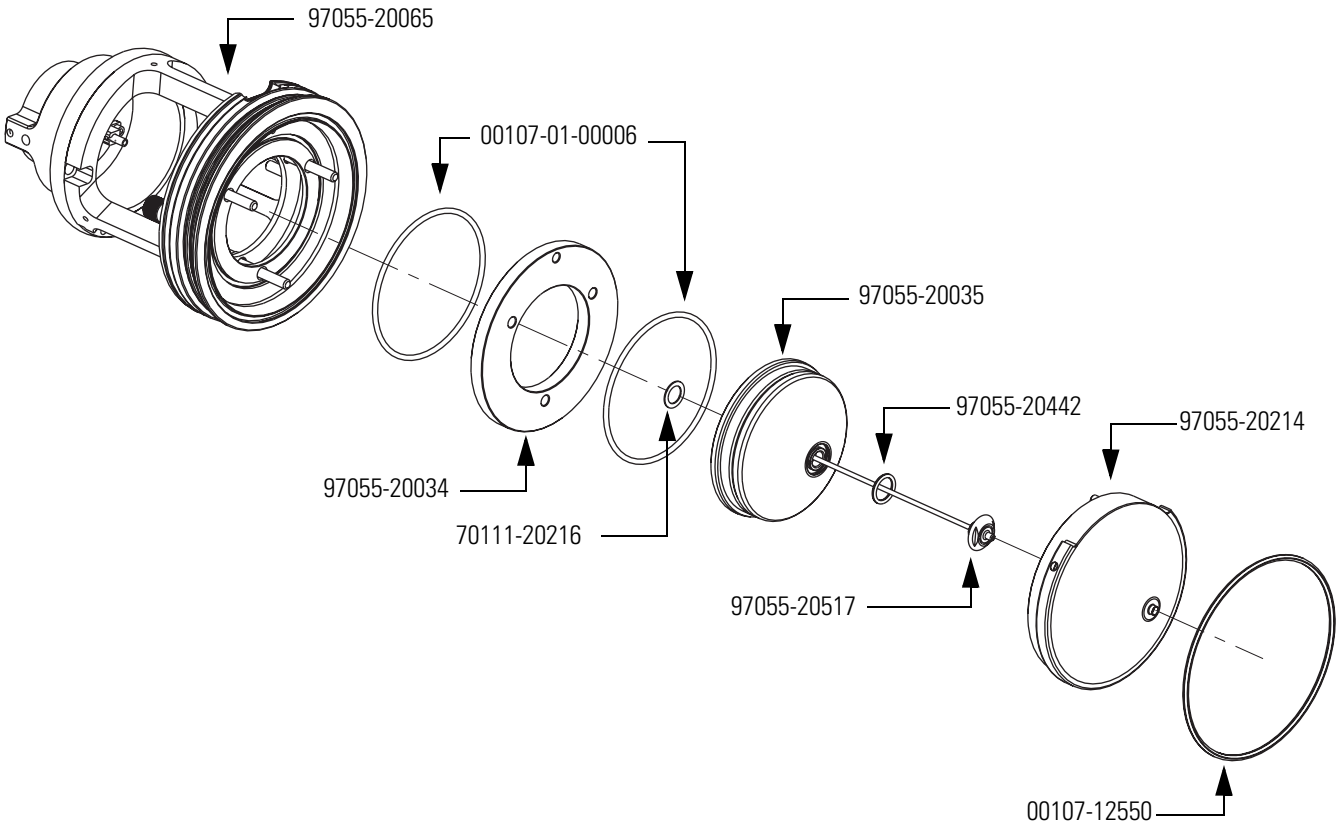
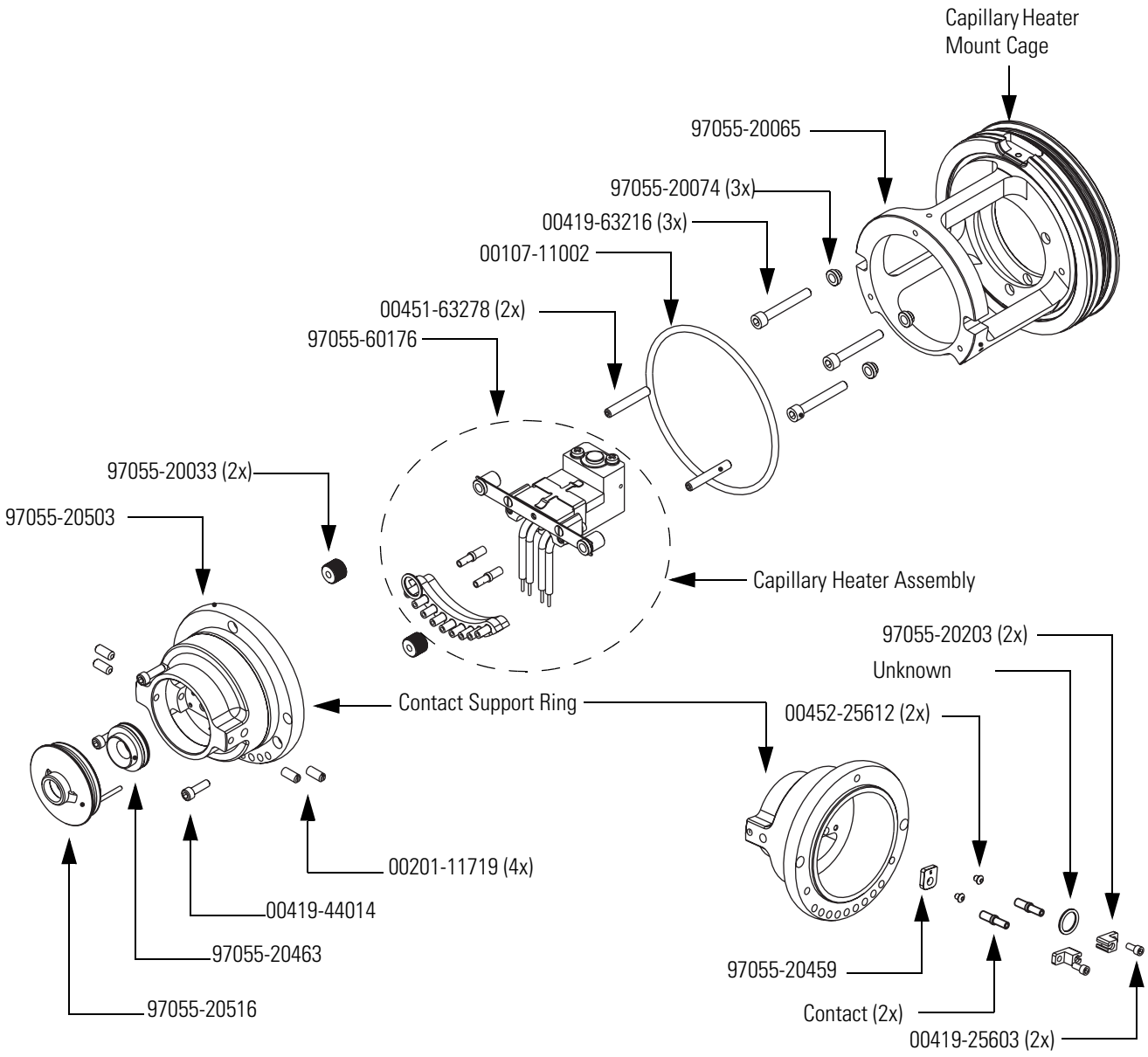


Figure 63. Ion source interface (back)



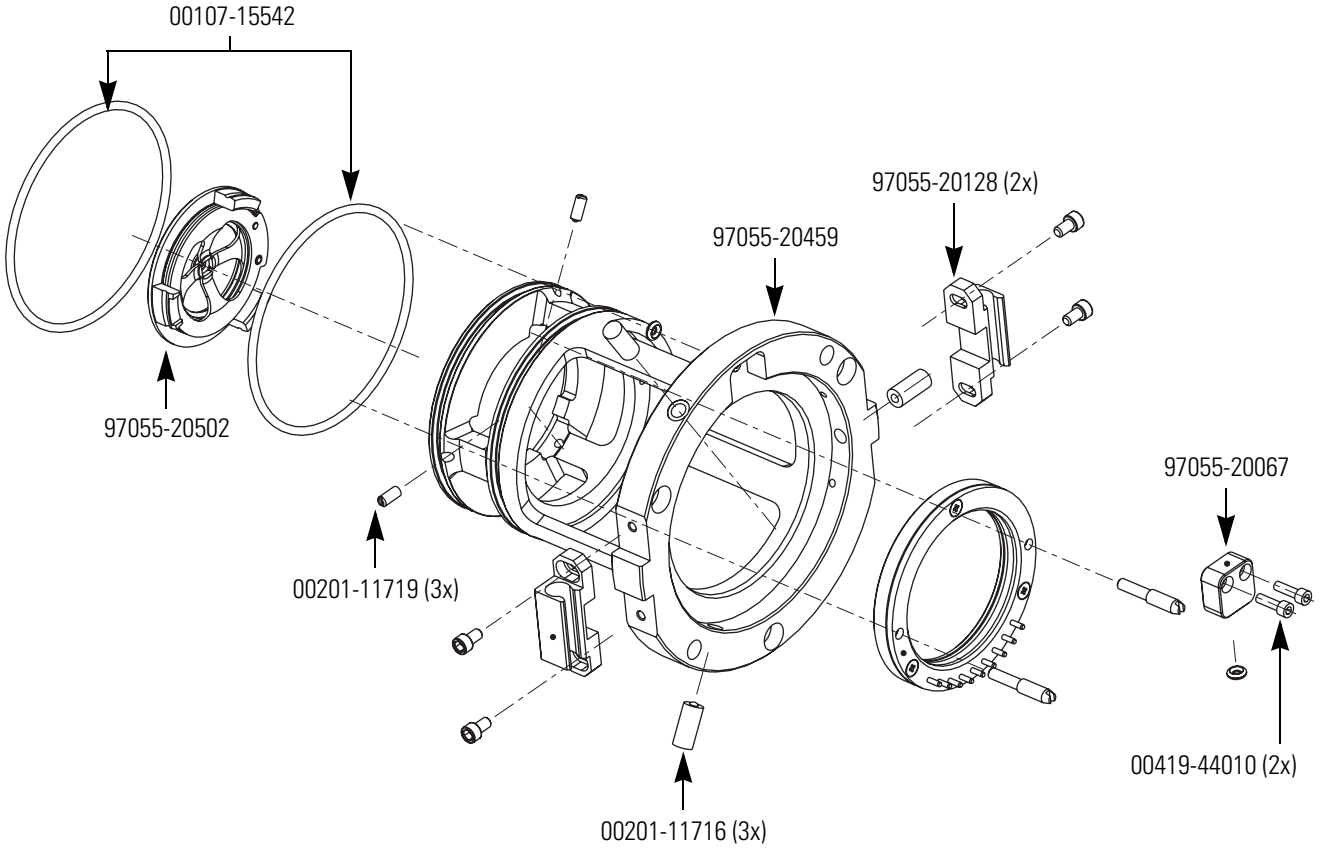
Q00 RF Lens

Figure 64 shows the replaceable parts for the Q00 RF lens.

Q00 Device Assembly 97055-60180

O-ring, 0.101-in. ID × 0.070-in. THK, Viton, ... 00107-02456
O-ring, 2.737-in. ID × 3/32-in. THK, Viton 884, ... 00107-15542
Plunger ball, ¼-20 × 0.53, 4lb, ... 00201-11716
Plunger ball, 6-40 × 0.31, 1lb, ... 00201-11719
Screw, socket HD, CAP, 4-40 × 3/8, stainless steel, ... 00419-44010
Cage, outer contact support, ... 97055-20459
Latch block, probe housing, ... 97055-20128
Device, Combo Q00/L0, ... 97055-20502

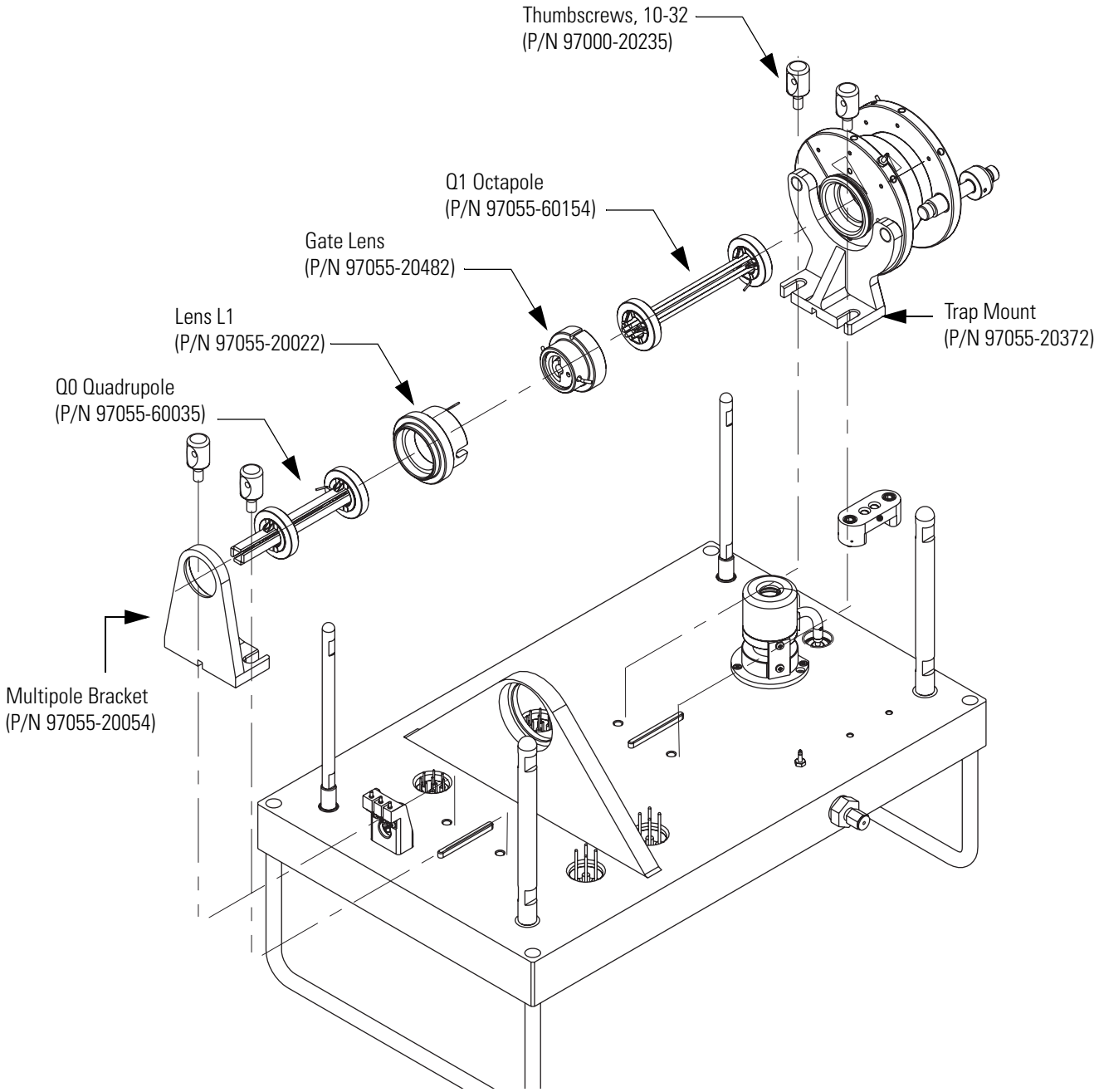
Figure 64. Q00 Device (RF Lens) part numbers



Q0 and Q1 Ion Guides

Thumb screws, 10-32,	97000-20235
Lens L1,	97055-20022
Gate lens,	97055-20482
Multipole bracket,	97055-20054
Q1 octapole,	97055-60154
Q0 quadrupole,	97055-60035
Trap Mount,	97055-20372

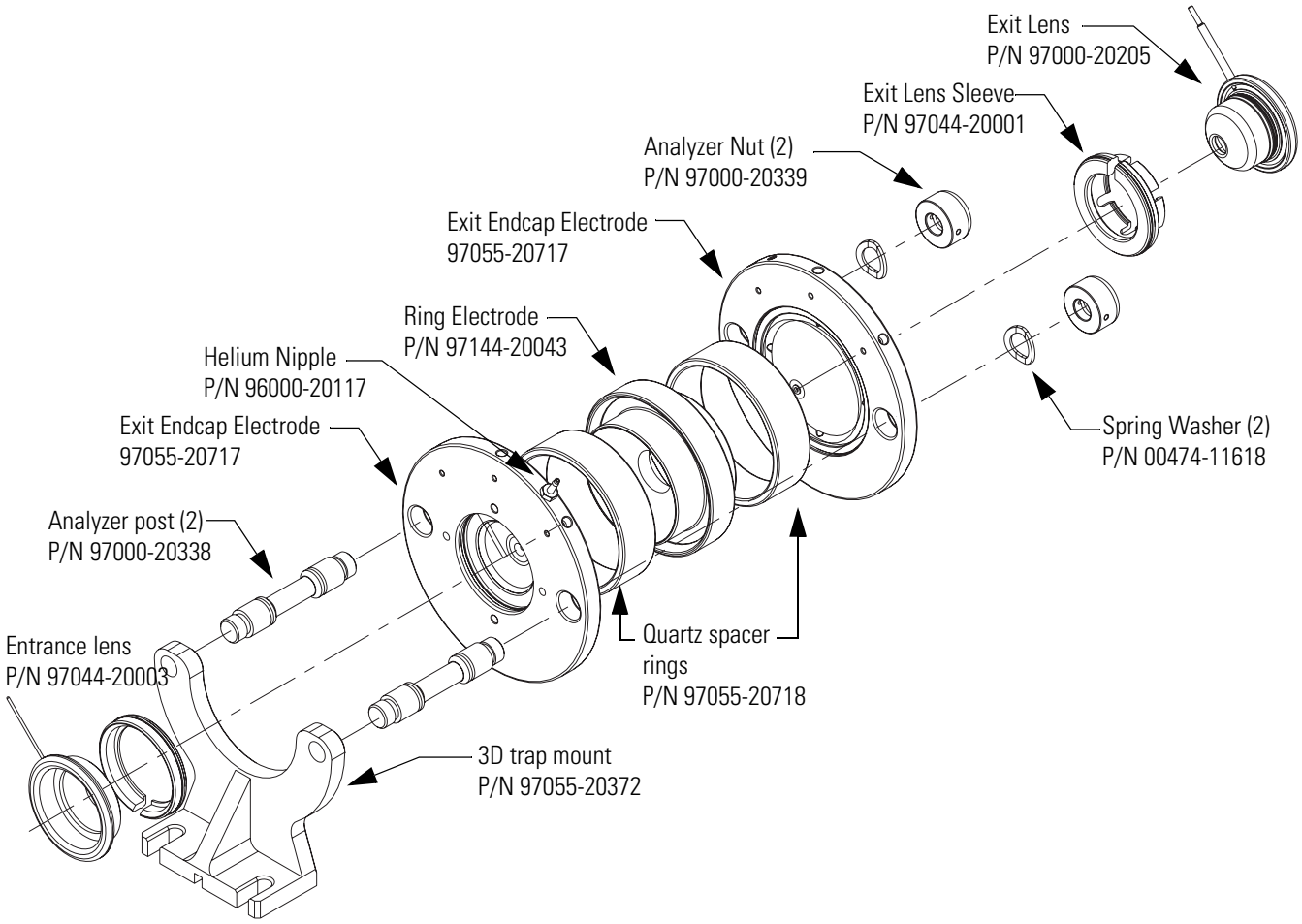
Figure 65. Q0 and Q1 ion guides part numbers



Mass Analyzer

Mass analyzer assembly, for Ultralite,	97055-60164
Mount, 3D trap	97055-20372
Post analyzer, LCQ	97000-20338
Endcap, tipped	97055-20717
Spacer, 3D trap	97055-20718
Electrode, RF ring, DE	97144-20043
Washer, spring, 0.33-in. ID × 0.49-in. OD, stainless steel	00474-11618
Nut, analyzer	97000-20339
Sleeve, exit lens	97044-20001
Exit lens	97000-20205
Sleeve, entrance lens	97044-20002
Entrance lens	97044-20003
Nipple, helium	96000-20117

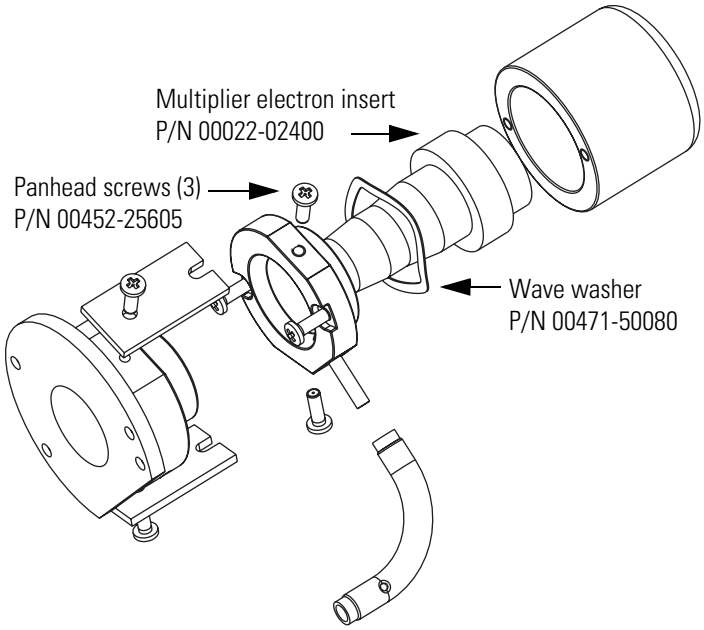
Figure 66. Mass analyzer exploded view



Electron Multiplier

Electron multiplier assembly,. 96000-60036
Multiplier, electron insert 00022-02400
Washer, wave, 0.731-in. OD × 0.588-in. ID, CS 00471-50080
Screw, panhead, 2-56 × 1/4-in., vented, stainless steel. 00452-25605

Figure 67. Assembly drawing of the electron multiplier



Coil Module

RF coil and PCB Assembly,. 97055-60218
Assembly, RF coil wound, 3D trap 97055-60217
Assembly, contact, RF detector, 10 kV 97055-60174

Divert/Inject Valve

Divert/inject valve (Rheodyne, 2 position, 6 port), ... 00110-03-00001
KIT, rebuild, divert six-port, 7900, LTQ. 00110-03-00002

Syringe Pump

Syringe pump,. 97055-98006

Turbomolecular Pump

Turbomolecular pump insert (Leybold TW 220/150/15),
(available as an exchange) EX00108-01-00004
Turbomolecular pump controller (Leybold TDS),. 00108-10012

Forepump

Forepump Kit, ... 70111-62014
Forepump (mechanical pump), E2M30,
650 L^3/min, 220V AC, (available as an exchange) 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
Clamp, high-torque, 1 1/4-in. to 2 1/8-in., stainless steel 00201-99-00056
PVC vacuum hose reinforced, 1.5-in ID, ... 00301-24163
Drain oil return kit, ... 00960-01-00007
Adapter, pump roughing line, ... 70111-20210

Pressure Gauges

Convectron gauge, ... 00105-00501
Kit, ion gauge, ... 97055-62001S

Vacuum Accessories

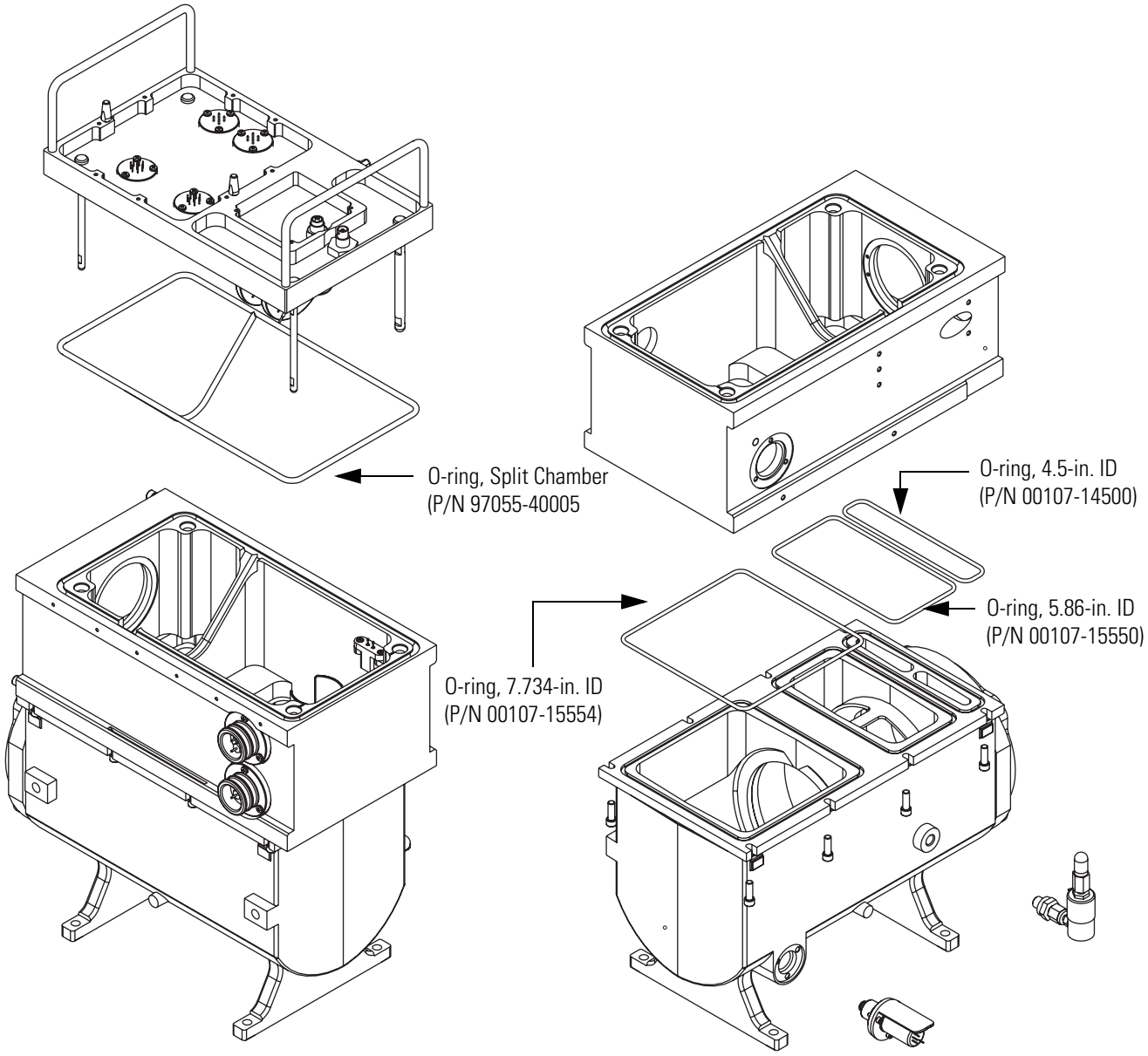
Hose and Accessories Kit, ... 97055-62007
PVC vacuum hose reinforced, 1.5-in. ID, ... 00301-24163
Adapter, for mechanical pump hose, NW-40 × 1.515-in. OD 97055-20714
Flange, NW40, long, ... 00108-02-00003
Clamp, NW32/40, swing, ... 00108-02-00004
Ring, centering, ... 00108-02-00005
Adaptor, pump roughing line, ... 70111-20210
Hose clamp, band, ... 00201-03810
Clamp, high-torque, 1.25-in. to 2.125-in., stainless steel 00201-99-00056
Pump hardware centering ring, ... 00108-02011
Vacuum hardware clamp KF-20/25, ... 00102-10020

Vacuum Manifold O-Rings

Figure 68 shows the vacuum manifold O-rings.

O-ring, 0.31-in. ID × 1/16-in. THK, Viton 00107-05000
O-ring, 4.5-in. ID × 1/8-in. THK, Viton, ... 00107-14500
O-ring, 6.48-in. ID × 1/8-in. THK, Viton, ... 00107-15270
O-ring, 7.734-in. ID × 1/8-in. THK, Viton, ... 00107-15544
O-ring, 5.86-in. ID × 1/8-in. THK, Viton, ... 00107-15550
O-ring, split chamber, ... 97055-40005

Figure 68. Vacuum pump O-rings



Vent Valve

Vent valve assembly, ... 97055-60084
O-ring, 0.468-in. ID × 0.078-in. THK, Viton 00107-07600
Fitting, swage, O-seal, 1/4-in. OD tube, 7/16-20 00101-13510
Fitting, swage, fractional tube adapter to male pipe, NPT, 1/4-in. OD tube, 1/8-in. male pipe size 00101-01740
Filter, sintered nylon 00201-06050
Ribbon dope, 1/4-in. 00301-16501
Valve, two-way, normal open, 24 V, 1 W, coil, 1/8-in. NPT 00110-02-00001

Power Supplies

PS1, +60 V (6 A), +5 V (35 A), ±15 V (14 A), ... 97055-60014
PS2, +36 V (10 A), ±24 V (8.5 A), +28 V (6.7 A), ... 97055-60015
8 kV Power Supply, mounted 97355-60003
15 kV dual Electron Multiplier/Conversion Dynode power supply,. 97055-98043
Assembly, AC power module, single mechanical pump 97055-60133
Assembly, I/O board, Endeavor. 97055-61070
PCB assembly, surge absorber 70005-61090
PCB assembly, interlock, Quantum. 70111-61060S
PCB assembly, adapter, L-connector, power module 97055-61080

Printed Circuit Boards (PCBs)

Source PCB (available as exchange), ... 70111-61053S
Interlock PCB, ... 70111-61060S
Digital PCB (available as exchange), ... 97055-61013S
Distribution PCB,. 97055-61025
Analog PCB (available as exchange), ... 97055-61033S
Top Cover PCB. 97355-61040S
I/O PCB, ... 97055-61070S
Front Panel PCB, ... 97055-61110
Electrometer PCB, ... 97055-61170S
Low Pass Filter/Balun PCB 97055-61421
Divert/Inject Valve PCB,. 97055-61140
RF Amplifier PCB, ... 97055-61180S
PCB assembly, surge absorber 70005-61090
PCB assembly, adapter, ELCON, PMOD. 97055-61080
Assembly, PCB, syringe control and status display. 97055-61414
Assembly, PCB, single detector 97055-61430
Assembly, PCB, RFA adapter 97055-61150

Cables

Ethernet (Power Module) to Digital PCB,. 00012-70064
Power Module wire set, ... 97055-63003
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
Power module, +36/-28 Volt RF Amp Inhibit, ... 97055-63010
Convectron gauge to Power/Signal Distribution PCB, ... 97055-63016
Status Display/ Front Panel, ... 97055-63018
Divert Valve PCB to Divert Valve,. 97055-63020
Manifold Flange to Power/Signal Distribution PCB,. 97055-63022
RF Detect Sport to Power/Signal Distribution PCB,. 97055-63024
RF Amplifier Control to Power/Signal Distribution PCB,. 97055-63026
RF Amplifier Power to Power/Signal Distribution PCB, ... 97055-63028
Source & Top Cover SPI to Power/Signal Distribution PCB, ... 97055-63030

Vent, Turbo & Fans to Power/Signal Distribution PCB, ... 97055-63032
Daisy, Cooling Fans (3), ... 97055-63033
Dual Dynode / Electron Multiplier Supply to
Power/Signal Distribution PCB, ... 97055-63037
Elcon, Power to Power/Signal Distribution PCB, ... 97055-63038
Elcon, System Signals to Power/Signal Distribution PCB, ... 97055-63040
PS2 to Elcon Connector, Sled, ... 97055-63042
PS1 to Elcon Connector, Sled, ... 97055-63044
Cable, molded RCA, straight-to-90 plug,1 97055-98108
Analog PCB to Top Cover PCB, ... 97055-63048
Interlock (AC Power Module) to Source PCB, ... 97055-63050
Turbomolecular pump, RS485 to Digital PCB, ... 97055-63052
Analyzer Electrometer to Digital PCB, ... 97055-63056
Coaxial, LPF to RF Amplifier, ... 97055-63060
RF Amp Modulation to RF Detector, ... 97055-63062

Fans

Fan, 100 CFM, 24V dc, located on fan housing assembly
and on the coil box, ... 00013-00243
Fan, 21 CFM, 24V dc, located adjacent
to the turbomolecular pump, ... 97055-63083
Fan filter, ... 97055-20254

Manuals

The following manuals for the LCQ Fleet MS detector are provided on the instrument control software CD.

- *LCQ Fleet Preinstallation Guide* (LCQFleet_Install.pdf)
- *LCQ Fleet Getting Connected Guide* (LCQFleet_Connect.pdf)
- *LCQ Fleet Getting Started Guide* (LCQFleet_Start.pdf)
- *LCQ Fleet Hardware Manual* (LCQFleet_Hardware.pdf)

❖ To open the PDF files

1. From the Windows XP Start menu, choose **All Programs > Xcalibur > Manuals > LCQ Fleet**.
2. Click the PDF for the manual that you want to view.

MS Accessory Kit

Kit, MS accessory 70111-62034
Container, shipping, accessory kit, large 70111-98271
Syringe, 500 µL, gas tight, removable needle, (2 each) 00301-19016
Tube, hypodermic, 28-gauge 00106-20000
Fuse, 1.00 A, 5x20, 250 V, quick acting 00006-07610
Fuse, 4 A, 5 × 20 mm, 250 V, time lag 00006-11420
Fuse, 0.16 A, 250 V, 5 × 20 mm 00006-01700
Fuse, 0.4 A, 250 V, 5 × 20 mm 00006-05080
Fuse, 0.25 A, 250 V, 5 × 20 mm 00006-11204
Fuse, 0.500 A, 250 V, 5 × 20 mm, quick acting 00006-07608
Fuse, 3.15 A, 250 V, 5 × 20 mm 00006-10510
Fuse, 6.3 A, 250 V, slo-blo, 5 × 20 mm, low breaking capacity, ROHS 00006-11450
Fuse, 1.0 A, 250 V, time lag, microfuse 00006-14015
Fuse, micro, 2 A, time lag, 250 V, short leads 00006-09102
Fuse, micro, 4 A, time lag, 250 V, short leads 00006-10705
Fitting, HPLC adapter, 10-32 × 1/4 PEEK 00101-18080
Fitting, ferrule, Swagelok, front, for 1/4-in. tubing (2 each) 00101-10000
Fitting, ferrule, Swagelok, back, 1/4 (2 each) 00101-04000
Fitting, ferrule, Swagelok, back, 1/8 (2 each) 00101-02500
Fitting, ferrule, Swagelok, front, 1/8 (2 each) 00101-08500
Septa, Supelco Thermogreen™, LB-1, 9.5 mm (3 each) 00301-16999
Fitting, nut, fingertight, HPLC,10-32, PEEK (3 each) 00101-18081
Fitting, HPLC, Tee, 0.02-in. orifice, PEEK 00101-18204
Fitting, HPLC,10-32, short 1-piece, 10/pkg, ROHS (6 each) 00109-99-00016
Fitting, Swagelok nut, for 1/8-in. OD tubing, brass (2 each) 00101-15500
Fitting, ferrule, for 1/8-in. OD tubing, short, Tefzel (2 each) 00101-18223
Seal, ring, graphite vespel 97055-20442
Ferrule, fingertight 2, Upchurch, (8 each) 00101-18196
Ferrule, 0.008-in. ID, Kel-F HPLC (4 each) 00101-18114
Fitting, fingertight 2, Upchurch (4 each) 00101-18195
Tubing, fused-silica, 0.150 mm × 0.390 mm (3 unit of length) 00106-10498
Tubing, fused-silica, 0.05-in. ID × 0.19-in. OD (3 ft. length) 00106-10502
Tubing, fused-silica, 0.10-in. ID × 0.19-in. OD (12 ft. length) 00106-10499
Syringe, adapter kit 70005-62011
Tubing, red PEEK, 0.005-in. ID × 1/16-in. OD (10 ft. length) 00301-22912
Tube, Teflon, 0.03-in. ID ×1/16-in. OD 00301-22915
Tool, capillary removal, Quantum 70111-20258
Fitting, Swagelok, nut, for 1/4-in. OD tubing, brass (2 each) 00101-12500
Needle, corona, APCI (3 each) 70005-98033
Adaptor, drain hose 70111-20971

Special LXQ/LCQ Fleet Trap Accessory Kit

This kit is shipped with the LXQ and the LCQ Fleet MS detectors.

Kit, Accessory, special for LXQ TRAP 97055-62045

Cable, assembly, adapter, LC/MS interconnect 97055-63070
Capillary, 500 µm, 4.87-in. length 97055-20517
Kit, chemicals, LCQ 97000-62042
Wrench, Allen/Hex, 1/4-in., BP/W-handle 00725-00022
Seal, standard needle, 5000 series 00950-00952
Needle, D point, 26 gauge, 2-in. length, 0.24-in. D washer 00950-00990
Container, shipping, accessory kit, small 70111-98272
Cable, assembly, adapter, LC/MS, LTQ/LXQ interconnect
(for the LTQ, LXQ, and LCQ Fleet MS detectors) 60053-63037

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, 0.008-in. ID, Kel-F 00101-18116
Fitting, Fingertight 2, Upchurch 00101-18195
Fitting, union, ZDV, 1/4-28, PEEK, black 00109-00304
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
Fitting, union, ZDV, 1/4-28, PEEK, black 00109-00304
Blunt-tip, 34-gauge, 30 µm ID, stainless steel needle 70111-20288

Fittings, Ferrules, Sample Loops, Unions, 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 (for syringe adapter assembly), ... 00301-22915

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

CAUTION Store and handle all chemicals in accordance with standard safety procedures. The Material Safety Data Sheets (MSDS) describing the chemicals being used are to be freely available to lab personnel for them to examine at any time.

Index

D

E

F

G

H

I

L

M

N

O

P

Q

R

S

T

V

W

Z