

# **LCQ Fleet**

# **Hardware Manual**

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Release history: Rev A, September 2015

Software version: Microsoft Windows 7 Professional (32-bit and 64-bit) SP1—Thermo Foundation<sup>™</sup> 2.0 and later, and Thermo Xcalibur 2.2 and later; Windows XP Workstation SP3—Foundation 1.0.2 SP2 or earlier, and Xcalibur 2.1 SP1 or earlier; Thermo LTQ Tune Plus 2.7.0 and later

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# **Preface**

The *LCQ Fleet Hardware Manual* describes the modes of operation and hardware components for the Thermo Scientific<sup>™</sup> LCQ<sup>™</sup> Fleet<sup>™</sup> Series mass spectrometers (MSs). It also provides the instruments' cleaning and maintenance procedures.

#### Contents

- Related Documentation
- Cautions and Special Notices
- Contacting Us

#### \* To suggest changes to the documentation or to the Help

Complete a brief survey about this document by clicking the button below. Thank you in advance for your help.



### **Related Documentation**

The LCQ Fleet mass spectrometer includes complete documentation. In addition to this guide, you can also access the following documents as PDF files from the data system computer:

- LCQ Fleet Preinstallation Requirements Guide
- LCQ Fleet Getting Connected Guide
- LCQ Fleet Getting Started Guide

- Ion Max and Ion Max-S API Source Hardware Manual
- Safety and Regulatory Guide

The LCQ Fleet also ships with a printed copy of the *Safety and Regulatory Guide*. This guide contains important safety information about Thermo Scientific liquid chromatography (LC) and mass spectrometry (MS) systems. Make sure that all lab personnel have read and have access to this document.

#### \* To view the product manuals

From the Microsoft<sup>™</sup> Windows<sup>™</sup> taskbar, choose **Start > All Programs > Thermo Instruments > Manuals > model**, where *model* is your specific model, and then open the PDF file to view it.

The LCQ Fleet application also provides Help.

#### ✤ To view the data system Help

- From the application window, choose **Help** from the menu bar.
- If information about setting parameters is available for a specific view, page, or dialog box, click **Help** or press the F1 key for information about setting parameters.

#### \* To download user documentation from the Thermo Scientific website

- 1. Go to www.thermoscientific.com.
- 2. In the Search box, type the product name and press ENTER.
- 3. In the left pane, select **Documents & Videos**, and then under Refine By Category, click **Operations and Maintenance**.
- 4. (Optional) Narrow the search results or modify the display as applicable:
  - For all related user manuals and quick references, click **Operator Manuals**.
  - For installation and preinstallation requirements guides, click **Installation Instructions**.
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### **Cautions and Special Notices**

Make sure you follow the cautions and special notices presented in this guide. Cautions and special notices appear in boxes; those concerning safety or possible system damage also have corresponding caution symbols.

This guide uses the following types of cautions and special notices.



**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 might contain information that is critical for optimal performance of the system.

**Note** Highlights information of general interest.

**Tip** Highlights helpful information that can make a task easier.

The LCQ Fleet Hardware Manual contains the following caution-specific symbols (Table 1).

 Table 1.
 Caution-specific symbols and their meanings (Sheet 1 of 2)

#### Symbol Meaning



**Chemical hazard:** Observe Good Laboratory Practices (GLP) when handling chemicals. Only work with volatile chemicals under a fume or exhaust hood. Wear gloves and other protective equipment, as appropriate, when handling toxic, carcinogenic, mutagenic, corrosive, or irritant chemicals. Use approved containers and proper procedures to dispose of waste oil and when handling wetted parts of the instrument.



**Hot surface:** Allow heated components to cool before touching or servicing the instrument.

| Symbol   | Meaning  |
|----------|--|
| <u>A</u> | <b>Risk of electric shock:</b> This instrument uses voltages that can cause electric shock and/or personal injury. Before servicing, shut down the instrument and disconnect it from line power. While operating the instrument, keep covers on. |
|          | <b>Risk of eye injury:</b> Eye injury could occur from splattered chemicals or airborne particles. Wear safety glasses when handling chemicals or servicing the instrument.  |
|          | <b>Sharp object:</b> Avoid handling the tip of the syringe needle or the corona needle that is located inside the API source.  |

#### Table 1. Caution-specific symbols and their meanings (Sheet 2 of 2)

## **Contacting Us**

There are several ways to contact Thermo Fisher Scientific for the information you need. You can use your smartphone to scan a QR code, which opens your email application or browser.

| Contact us | <b>Customer Service and Sales</b>                | Technical Support                           |
|------------|--|---|
|            | (U.S.) 1 (800) 532-4752                          | (U.S.) 1 (800) 532-4752                     |
|            | (U.S.) 1 (561) 688-8731                          | (U.S.) 1 (561) 688-8736                     |
|            | us.customer-support.analyze<br>@thermofisher.com | us.techsupport.analyze<br>@thermofisher.com |
|            |  |   |

| Contact u   | S                    | <b>Customer Service and Sales</b>   | Technical Support                    |  |
|---|----------------------|---|--------------------------------------|--|
|   | *                    | To find global contact information  | or customize your request            |  |
|   | 1.                   | Go to www.thermoscientific.com.   |                                      |  |
|   | ■ <sup>2.</sup><br>Ç | Click <b>Contact Us</b> , select the <b>Using/</b> type the product name. | Servicing a Product option, and then |  |
|   | 3.                   | Use the phone number, email addre   | ess, or online form.                 |  |
| To find product support, knowledge bases, and resources |                      |   |                                      |  |
|   |                      | Go to www.thermoscientific.com/su   | ipport.                              |  |
|   | *                    | To find product information   |                                      |  |
|   |                      | Go to www.thermoscientific.com/lc   | e-ms.                                |  |
| Note To   | o provic             | le feedback for this document:  |                                      |  |
| • Sence   | l an em              | ail message to Technical Publications                                     | s (techpubs-lcms@thermofisher.com).  |  |
| • Complete a survey at www.surveymonkey.com/s/PQM6P62.  |                      |   |                                      |  |
|   |                      |   |                                      |  |

Preface

#### 1

# Introduction

The LCQ Fleet mass spectrometer (see Figure 1) is a member of the Thermo Scientific family of mass spectrometers. The LCQ Fleet is a 3D quadrupole ion trap mass spectrometer that includes a syringe pump, a divert/inject valve, and an Ion Max-S<sup>™</sup> API source. For descriptions of the various hardware components, see Chapter 2, "Functional Description."

**Note** The Glossary defines some of the terms used in this manual.



Figure 1. LCQ Fleet MS with the Ion Max-S API source

In a typical liquid chromatography/mass spectroscopy (LC/MS) analysis, the LC portion of the system separates a mixture into its chemical components. 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 LCQ Fleet MS where they are ionized and analyzed. As the instrument 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 instrument can also supply structural and quantitative information by performing MS<sup>n</sup> experiments.

Because the instrument has a built-in syringe pump and divert/inject valve, it provides four additional ways to introduce a sample into the instrument. See Table 2.

| Method                   | Description  |
|--------------------------|--|
| Automated loop injection | Connect a sample loop, an LC pump, and the syringe pump<br>to the divert/inject valve. After you connect the plumbing,<br>specify the flow rate at which the syringe pump fills the<br>sample loop. After the loop is filled, the data system triggers<br>an injection.                                |
| High-flow infusion       | Use a union tee to combine the flow from the syringe pump<br>with the flow from an LC pump.  |
| Infusion                 | Connect the built-in syringe pump directly to the atmospheric pressure ionization (API) source of the instrument.  |
| Manual loop injection    | Connect a sample loop, a needle port fitting, and an LC<br>pump to the divert/inject valve. After you fill the sample loop<br>with sample, switch the position of the divert/inject valve,<br>which places the contents of the sample loop in the path of<br>the solvent flow produced by the LC pump. |

 Table 2.
 Introducing samples into the instrument

The instrument consists of an API source, ion optics, a mass analyzer, and an ion detection system. The ion optics, mass analyzer, ion detection system, and part of the API source are enclosed in a vacuum manifold.

Ionization of the sample takes place in the API source. The specific method used to ionize the sample is referred to as the ionization technique. The 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 instrument to analyze positively or negatively charged ions or to switch between these polarity modes during a single run.

Certain 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<sup>TM</sup> (AGC) process 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 display and analysis by the data system.

The data system serves as the user interface to the instrument, autosampler, LC, and syringe pump. Refer to the data system Help for more information about the LCQ Fleet data processing and instrument control application.

Each sequence of loading the mass analyzer with ions followed by mass analysis of the ions is called a scan. The instrument 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, provides greater flexibility in the instrumentation for solving complex analytical problems.

For information about the electrospray (ESI) and atmospheric pressure chemical ionization (APCI) techniques, refer to the *Ion Max and Ion Max-S API Source Hardware Manual*. For information about the atmospheric pressure photoionization (APPI) technique, refer to the *Ion Max APPI Source User Manual*. For more information about the nanoelectrospray (nanoESI or NSI) technique, refer to the manual that came with your NSI source.

#### 1 Introduction

# **Functional Description**

This chapter describes the principal components of the LCQ Fleet MS and their functions.

#### Contents

- Overview
- Syringe Pump
- Divert/Inject Valve
- Mass Spectrometer

### **Overview**

Figure 2 shows a functional block diagram of an LCQ Fleet system that uses either a liquid chromatograph with an autosampler or the syringe pump as the inlet. A sample transfer line connects the LC to the mass spectrometer. The autosampler and LC are usually installed to the left of the instrument. The divert/inject valve is integrated into the front panel of the instrument.

In a typical analysis by LC/MS, a sample is injected onto an LC column. The sample then separates into its various components. The components elute from the LC column and pass into the instrument for analysis.

You can use any of these methods to ionize and desolvate sample molecules into the gas phase when they enter the atmospheric pressure ionization (API) source:

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

2

The ion optics focus and accelerate the resulting gas-phase sample ions into the mass analyzer, where they are isolated and ejected according to their mass-to-charge ratios. As the mass analyzer ejects the sample ions, a detection system detects them, which includes an electron multiplier that produces a signal proportional to the number of ions detected. The system electronics receive and amplify the ion current signal from the ion detection systems. The signal then passes on to the data system for further processing, storage, and display. The data system provides the primary mass spectrometer user interface.

Figure 2. Functional block diagram of an LCQ Fleet system



### **Syringe Pump**

The LCQ Fleet MS includes an electronically controlled, integrated syringe pump (see Figure 3). The syringe pump delivers sample solution from the syringe into the API source.



When the syringe pump is operating, a motor drives the pusher block that depresses the plunger of the syringe at a user-selectable rate. Liquid flows out of the syringe needle and into the sample transfer line as the plunger is depressed. A syringe holder holds the syringe in place.

For instructions about setting up the syringe pump, refer to the *LCQ Fleet Getting Started Guide*.

#### Syringe Pump On/Off Button

The blue button located on the front panel above the syringe pump (Figure 4) turns the syringe pump on and off. The motor has two speeds: normal and fast. The normal speed produces the flow rate specified in the data system. Pressing and releasing the button turns on the syringe pump and sets the motor speed to the normal speed. When you press and hold the button down, the motor moves the pusher block at the fast speed. The motor maintains the fast speed until you release the button or the pusher block reaches the end of its path. When you release the button, the pusher block slows to normal speed. Pushing the button a second time turns off the syringe pump.



**Figure 4.** Syringe pump on/off button

#### **Syringe Pump LED**

A light-emitting diode (LED) to the right of the on/off button indicates whether the pump is on or off. Table 3 lists the states of the syringe pump LED.

**Table 3.** Syringe pump LED states

| State           | Meaning   |
|-----------------|---|
| Not illuminated | The syringe pump is off.  |
| Steady green    | The syringe pump is on. The pusher block is moving at a normal<br>speed that produces the flow rate specified in the data system. The<br>allowable flow rate setting depends on the syringe size. |
| Flashing green  | The syringe pump is on and the pusher block is moving at the fast speed.  |

### **Divert/Inject Valve**

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

You can configure (plumb) the divert/inject valve in one of two ways: as a divert valve for direct infusion, high-flow infusion, or LC/MS experiments; or as a loop injector for flow-injection analysis. For procedures about plumbing the valve in the loop injector or configuring the divert valve, refer to the *LCQ Fleet Getting Started Guide*.

You can use the divert/inject valve button or the data system to control the divert/inject valve. Refer to the data system Help for instructions about operating the divert/inject valve.

#### **LEDs and Button**

The control button for the divert/inject valve is located on the front panel to the right of the divert/inject valve. It switches the valve between two positions. The LEDs to the left of the button indicate the position of the valve (Figure 5).





When the divert/inject valve is set up for loop injections (flow injection analysis [FIA]), pressing the divert/inject valve button switches 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 switches the LC flow between the instrument and the waste container. The Detector and Waste LEDs indicate the position of the valve.

#### **Divert Valve Positions**

Use the divert/inject valve to divert the solvent flow between the instrument and the waste container (Figure 6). The divert valve has two positions:

- Detector position—Solvent flow from the LC pump enters the valve through port 2 and exits through port 3 to the union tee.
- Waste position—Solvent flow from the LC pump enters the valve through port 2 and exits through port 1 to the waste container.



Figure 6. Divert valve positions

#### **Injection Valve Operation**

In the loop injection configuration (Figure 7), use the divert/inject valve button to switch between load and inject modes. The injector valve has two positions:

- Load position—The injected sample enters the valve through port 5 and exits the sample loop through ports 4 and 1, respectively. As you overfill the sample loop, the sample solution exits the valve through port 6. Solvent flow from the LC pump enters and exits the valve through ports 2 and 3, respectively.
- Inject position—After you fill the sample loop, press the blue button above the injection valve or use the controls available in Tune Plus. Solvent flow from the LC pump backflushes sample out of the sample loop and then out of the valve through port 3 toward the detector.



### **Mass Spectrometer**

The LCQ Fleet MS provides sample ionization and mass analysis of injected samples or samples eluted from a liquid chromatograph. The instrument uses a 3D quadrupole ion trap mass analyzer with an API source that is external to the mass analyzer.

The instrument includes the following components:

- LEDs
- Power Panel
- API Source
- Ion Optics
- Mass Analyzer
- Ion Detection Systems
- Vacuum System
- Inlet Gases Hardware
- Cooling Fans

### LEDs

Figure 8 shows the LEDs on the instrument's front panel with their descriptions listed in Table 4.

Figure 8. LCQ Fleet front panel LEDs



| LED           | State         | Description  |
|---------------|---------------|--|
| Power         | Green         | Power is being supplied to the instrument. (The electronics service switch is in the Electronics Normal position.)     |
|               | Off           | Power is not being supplied to the instrument.<br>(The electronics service switch is in the Service<br>Mode position.) |
| Vacuum        | Yellow        | The vacuum is outside the allowable operating range.   |
|               | Green         | The vacuum is within the allowable operating range.  |
| Communication | Yellow        | The instrument and data system are trying to establish a communication link.   |
|               | Green         | The instrument and data system are communicating.  |
| System        | Yellow        | The instrument is in standby mode.   |
|               | Green         | The instrument is on.  |
|               | Off           | The instrument is off.   |
| Scanning      | Flashing blue | The instrument is on and scanning.   |
|               | Off           | The instrument is not scanning.  |

#### Table 4. LCQ Fleet status LEDs

### **Power Panel**

The power panel (Figure 9) is located on the right side of the instrument.





The instrument receives line power at 230 Vac  $\pm$  10%, 50/60 Hz, 10 A through the right-side power panel. The power panel provides system power control, a contact closure interface (Peripheral Control), an Ethernet 100Base-T connection from the instrument to the data system computer, and a system Reset button. The power panel accepts line power, filters it, and provides it to various components of the instrument.

#### **Main Power Switch**

In the Off position, the Main Power (circuit breaker) switch removes all power to the instrument, including the external forepump. In the On position, power is supplied to the instrument. In the standard operational mode, the switch stays in the On position.



**CAUTION** In an emergency, do not use the electronics service switch to shut off power to the mass spectrometer. Instead, place the main power circuit breaker switch (labeled *Main Power*) in the Off (down) position.

#### **Electronics Service Switch**

The electronics service switch is a circuit breaker. In the Service Mode position, the switch removes power to all components of the instrument except for the fans and vacuum system. This setting allows you to service nonvacuum system components with the vacuum system still operating. In the Electronics Normal position, all components of the instrument have power.

#### **Reset Button**

When you briefly press the reset button, the embedded processing system and digital circuitry reset and the system software reloads from the data system. For information about resetting the instrument, see "Resetting the Mass Spectrometer" on page 34.

#### **API Source**

The 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 instrument. You can operate the API source in the ESI, H-ESI, NSI, APPI, or APCI mode.

For more information about the API source, refer to Chapter 2, "Setting Up the API Source," in the *LCQ Fleet Getting Started Guide*.

#### **API Source Interface**

The API source interface for the LCQ Fleet MS consists of the components of the API source that are held under vacuum (except for the atmospheric pressure side of the ion sweep cone) in a vacuum chamber that the forepump evacuates. The API source interface includes an ion sweep cone, an ion transfer tube, two cartridge heaters, a heater block, a sensor, an API tube lens, a skimmer, and a vent prevent ball (Figure 10). The tube lens and skimmer mount to the API source interface cage (Figure 11).

The ion sweep cone is a metal cone over the API ion transfer tube. The ion sweep cone acts as a physical barrier that protects the entrance of the ion transfer tube and increases source robustness.

The ion transfer tube is a metal, cylindrical tube that assists in desolvating ions produced by the API probe while transferring them into the vacuum system.

The heater block contains two heater cartridges, surrounds the ion transfer tube, and heats the tube to temperatures up to 400 °C (752 °F). A probe sensor measures the temperature of the heater block. A decreasing pressure gradient draws ions into the ion transfer tube in the atmospheric pressure region and transports them to the ion transfer tube–skimmer of the vacuum manifold. The vent prevent ball stops air from entering the vacuum manifold when the tube is removed so that you can remove the ion transfer tube for cleaning without venting the system.



# **Figure 10.** API source interface (cross section)

Figure 11. Internal (under vacuum) components of the LCQ Fleet MS



Ions from the ion transfer tube enter the tube lens (Figure 12). The API tube lens offset voltage applied to the tube lens accelerates the ions into the background gas that is present in the ion transfer tube–skimmer region. Collisions with the background gas aid in the desolvation of the ions and increase sensitivity. However, if the tube lens offset voltage is too high, collisions with the background gas can be energetic enough to cause ion fragmentation. This fragmentation, or collision-induced dissociation (CID), in the ion transfer tube–skimmer region decreases sensitivity. Therefore, when you tune the instrument, 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 API source interface region and the lower pressure Q00 rf lens region of the vacuum manifold.

Figure 12. Skimmer and tube lens (back view)



#### **Ion Optics**

The following ion optics focus the ions produced in the API source and transmit them to the mass analyzer:

- Q00-L0 RF Lens
- Q0 Ion Optics
- Q1 Ion Optics

#### **Q00-L0 RF Lens**

The Q00-L0 rf lens is located closest to the API source. The Q00-L0 device includes the Q00 rf lens and the lens L0.

The square-metal elements of the Q00 rf lens act as an ion-focusing device. An rf voltage that is applied to the elements creates an electric field that guides the ions along the axis of the lens. A dc voltage offset from ground that is applied to multipole Q00 (called the Q00 offset voltage) increases the translational kinetic energy of the ions that emerge from the skimmer. During ion focusing, 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.

| The lens L0 is a metal plate with a small circular hole through which the ion beam passes.    | А    |
|---|------|
| potential is applied to lens L0 to aid in ion transmission. Lens L0 also acts as a vacuum baf | ffle |
| between the multipole Q00 and Q0 ion optics chambers.   |      |

#### **QO Ion Optics**

The Q0 ion optics transmit ions from the Q00 rf lens to the Q1 ion optics. The Q0 ion optics include multipole Q0 and lens L1.

The square-profile rods of the multipole Q0 act as an ion transmission device similar to the Q00 rf lens. An rf voltage that is applied to the rods creates an electric field that guides the ions along the axis of the multipole. The Q0 offset voltage increases the translational kinetic energy of ions that emerge from Q00.

The lens L1 is a metal plate with a small circular hole in the center through which the ion beam passes. An electrical potential applied to the lens accelerates (or decelerates) ions as they approach the lens. This electrical potential focuses the ion beam as it passes through the lens. Lens L1 also acts as a vacuum baffle between the Q0 ion optics chamber and the mass analyzer chamber.

#### **Q1 Ion Optics**

The Q1 ion optics transmit ions from the Q0 ion optics to the mass analyzer. The Q1 ion optics include Q1 and the split gate lens.

Multipole Q1 is an array of circular rods that act as an ion transmission device similar to multipole Q0. An rf voltage that is applied to the rods creates an electric field that guides the ions along the axis of the multipole. The Q1 offset voltage increases the translational kinetic energy of ions that emerge from Q0.

A split gate lens starts and stops the injection of ions into the mass analyzer by deflecting the beam at high speeds at the appropriate times.

#### **Mass Analyzer**

The mass analyzer is the site where ion manipulation and mass analysis occur, which includes ion storage, ion isolation, CID, and ion ejection. This section describes the components of the mass analyzer, voltages applied to the mass analyzer electrodes, the presence of helium damping gas in the mass analyzer cavity, and mass analyzer operation during mass analysis.

- Components
- Main RF Voltage Applied to the Mass Analyzer Ring Electrode
- AC Voltages Applied to the End Caps
- Helium Damping Gas
- Summary of Mass Analyzer Operation

#### **Components**

The mass analyzer consists of an entrance endcap electrode closest to the ion optics, a ring electrode between the two endcap electrodes, and the exit endcap electrode, which is closest to the ion detection system (Figure 13). Both endcap electrodes have metal disks with small circular holes in their centers through which ion beams pass into and out of the mass analyzer. The inner surfaces of these electrodes form a cavity in which mass analysis occurs.

Ions produced in the API source enter the mass analyzer cavity through the entrance endcap electrode. Ions eject through either endcap electrode during mass analysis. The conversion dynode accelerates ions ejected from the exit endcap toward 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.

#### Figure 13. 3D ion trap assembly



#### Main RF Voltage Applied to the Mass Analyzer Ring Electrode

The rf voltage is applied only to the ring electrode and is of constant frequency (825 kHz) and variable amplitude (0–10 000 V zero-to-peak). Because the frequency of this rf voltage is in the rf range, it is referred to as the main rf voltage. Applying 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 conversion dynode (Figure 13 on page 17). 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.

Low amplitude of the main rf voltage traps all ions above a minimum mass-to-charge ratio. This rf voltage is referred to as the storage voltage, and the minimum mass-to-charge ratio selected by the mass spectrometer is usually 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 Da/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 the mass analyzer ejects them. The voltage at which the mass analyzer ejects an ion is defined as its resonance voltage. The ejection of ions at each mass-to-charge ratio occurs over a very short time with the ion detection system detecting many of these ejected ions.

#### **AC Voltages Applied to the End Caps**

The mass spectrometer applies ion isolation waveform voltage, resonance excitation ac voltage, and resonance ejection ac voltage to the end caps to stimulate motion of the ions in the direction of the ion detection system. When the ac frequency applied to the end caps equals the frequency of the motion of the 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 mass analyzer ejects the ion in the direction of the ion detection system (X direction).

The ion isolation waveform voltage is a multifrequency resonance ejection waveform that acts during the ion isolation step of SIM, SRM, CRM, or  $MS^n$  (n > 1) full-scan applications. The ion isolation waveform voltage, combined 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.
During the CID step of SRM, CRM, or  $MS^n$  (n > 1) full-scan applications, the mass spectrometer applies a resonance excitation ac voltage to the end caps to fragment precursor ions into product ions. This step enhances ion motion and the ion gains kinetic energy. After many energetic collisions with the helium damping gas, which is present in the mass analyzer, the ion gains enough internal energy to cause it to dissociate into product ions. The product ions are then mass analyzed.

During ion scan-out, the resonance ejection ac voltage assists in the ejection of ions from the mass analyzer, which improves mass resolution and sensitivity. The mass spectrometer applies resonance ejection ac voltage during the ramp of the main rf voltage. Ions consecutively move into resonance with the resonance ejection ac voltage. When an ion approaches resonance, it moves farther away from the center of the mass analyzer, which subsequently ejects it.

### **Helium Damping Gas**

The mass analyzer cavity contains helium that is used as a damping gas and a collision activation partner. The collisions of the ions that enter the mass analyzer with the helium slow the ions so that the rf field in the mass analyzer can more efficiently trap them.

The presence of helium in the mass analyzer cavity significantly enhances sensitivity and mass spectral resolution. Before their ejection from the mass analyzer cavity, sample ions collide with helium atoms. These collisions reduce the kinetic energy of the ions, which results in damping the amplitude of their oscillations. The ions are then focused to the axis of the cavity rather than allowed to spread throughout the cavity, which would spread their ejection times and degrade the mass spectral resolution.

Helium in the mass analyzer cavity also serves as a collision activation partner. During the CID step of SRM, CRM, or  $MS^n$  (n > 1) full-scan analysis, the mass spectrometer applies the resonance excitation ac voltage to the exit rods. This drives precursor ions energetically into the helium atoms. After gaining sufficient internal energy from the resulting collisions, the precursor ion dissociates into one or more product ions.

### **Summary of Mass Analyzer Operation**

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

- 1. Ion storage
- 2. Ion isolation (SIM, SRM, CRM, or  $MS^n$  [n > 1] full scan only)
- 3. CID (SRM, CRM, or  $MS^n$  [n > 1] full scan only)
- 4. Ion scan-out (the ion detection step)

For SRM and MS/MS full-scan applications, the mass analyzer performs the ion isolation and CID steps one time. For CRM and MS<sup>n</sup> (n > 1) full-scan applications, the ion isolation and CID steps are performed n - 1 times.

For SIM, SRM, CRM, or  $MS^n$  (n > 1) full scans, the mass spectrometer applies the ion isolation waveform voltage 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.

For SRM, CRM, or  $MS^n$  (n > 1) full-scan analyses, the mass spectrometer applies the resonance excitation ac voltage to the end caps to cause CID. The instrument does not store product ions with a mass-to-charge ratio of less than the minimum storage mass-to-charge ratio.

Finally, the sample ions or product ions are scanned out. The main rf voltage ramps up from low voltage to high voltage, and simultaneously the mass spectrometer applies the resonance ejection ac voltage 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 eject through the slots in the exit rods. Most of these ions are focused toward the ion detection system where they are detected.

### **Ion Detection Systems**

The LCQ Fleet MS has a high-sensitivity, on-axis ion detection system (Figure 14). The ion detection system produces a high signal-to-noise ratio (S/N) and enables voltage polarity switching between positive ion and negative ion modes of operation. The ion detection system is located behind the mass analyzer.

The conversion dynode is a concave metal surface located at a right angle to the ion beam. The instrument applies a high positive potential (15 kV) for negative-ion detection or a high negative potential (-15 kV) for positive-ion detection to the conversion dynode, which results in high conversion efficiency and increased signal. An ion striking the surface of the conversion dynode produces many secondary particles. The curved surface of the conversion dynode focuses these secondary particles and the 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 increase in conversion efficiency is more pronounced for more massive ions than for less massive ions.

The electron multiplier mounts on the top cover plate of the vacuum manifold next to the mass analyzer. The electron multiplier amplifies the signal and includes an anode that collects the electrons produced by the cathode. The data system records the combined current that leaves the electron multiplier through an anode.





### **Vacuum System**

The vacuum system evacuates the region around the API stack, ion optics, mass analyzer, and ion detection system. The vacuum system includes the following components (Figure 15):

- Vacuum Manifold
- Turbomolecular Pump
- Forepump
- Convectron Gauge
- Ion Gauge





### Vacuum Manifold

The vacuum manifold (Figure 16) encloses the API source interface, ion optics, mass analyzer, and ion detection system assemblies. The vacuum manifold is a thick-walled, aluminum chamber with a removable top cover plate, 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 16. Vacuum manifold with top cover plate and turbomolecular pump



### **Turbomolecular Pump**

A triple-inlet turbomolecular pump (Figure 17) provides the vacuum for the Q00 rf lens, Q0 ion optics, and analyzer regions of the vacuum manifold. The turbomolecular pump mounts under the vacuum manifold.





The Main Power switch turns off the turbomolecular pump. The electronics service switch has no effect on this pump. Power to the turbomolecular pump automatically shuts off if the turbomolecular pump's temperature becomes too high.

The turbomolecular pump sends status information, such as its temperature or rotational speed, to the data system computer.

### Forepump

The forepump creates the vacuum necessary for the proper operation of the turbomolecular pump. The forepump also evacuates the ion transfer tube region of the vacuum manifold.

The nondetachable power cord of the forepump plugs into the auxiliary power outlet labeled *Forepump* on the power panel (Figure 9 on page 12). The Main Power switch controls this outlet, not the electronics service switch.



**CAUTION** Always plug the forepump power cord into the power outlet labeled *Forepump* on the right side of the instrument. Never plug it into a wall outlet.

### **Convectron Gauge**

The Convectron gauge measures the pressure in the ion transfer tube in the vacuum manifold and the foreline, which connects the turbomolecular pump and the forepump. The source printed circuit board (PCB) monitors the pressure measured by the vacuum gauge.

#### Ion Gauge

An ion gauge measures the pressure in the analyzer region of the vacuum manifold and is also used for vacuum protection. Figure 17 on page 24 shows the ion gauge port.

### **Inlet Gases Hardware**

The inlet gas hardware controls the flow of damping gas, sheath gas, auxiliary gas, sweep gas, and air (during venting) into the instrument.

### **Vent Valve**

The vent valve (Figure 17 on page 24) allows the vacuum manifold to be vented to air that has been filtered through a sintered nylon filter. The vent valve, a solenoid-operated valve, is closed when the solenoid is energized.

The vacuum manifold vents when the instrument no longer receives external power, as with a power failure or by turning off the Main Power switch. Power is briefly provided to the vent valve after losing external power to protect against the accidental loss of power. When power to the vent valve solenoid shuts off for more than a very brief period of time, the vent valve opens and the manifold vents to filtered air.

### **Damping Gas Inlet Assembly**

The damping gas inlet assembly controls the flow of helium into the mass analyzer cavity. Helium (275  $\pm$ 70 kPa [40  $\pm$ 10 psi], 99.999% ultra-high purity) enters the instrument through a 1/8 in. port on the back of the instrument. The instrument regulates the flow of helium and delivers it to the mass analyzer.

Helium in the mass analyzer cavity dampens ionic motion and improves the performance of the instrument. See "Helium Damping Gas" on page 19.

### Sheath Gas, Auxiliary Gas, and Sweep Gas Valves

The sheath gas, auxiliary gas, and sweep gas valves control the flow of nitrogen into the API source (Figure 15 on page 22). Sheath gas is the inner coaxial nitrogen gas of the API probe that sprays (nebulizes) the sample solution into a fine mist as it exits the sample tube. Auxiliary gas is the outer coaxial nitrogen gas that assists the sheath gas in nebulizing and evaporating sample solutions. Sweep gas flows out from behind the sweep cone in the API source interface. Sweep gas aids in solvent declustering and adduct reduction.

Dry nitrogen (690  $\pm$ 140 kPa [100  $\pm$ 20 psi], 99% high purity) enters the instrument through a 1/4 in. port on the back of the instrument. The data system controls the valves that regulate the nitrogen pressure. You can set the flow rates from the Tune Plus window.

### **Cooling Fans**

Five fans provide internal cooling for the LCQ Fleet MS. Cooling air enters through the main air intake fans on the back of the mass spectrometer. Exhaust air exits the instrument from the side ventilation slots.



**CAUTION** To ensure safety and proper cooling, always operate the mass spectrometer with its covers in place. This is also necessary to comply with product safety and electromagnetic interference regulations.

# 3

# System Shutdown, Startup, and Reset

Many maintenance procedures for the LCQ Fleet system require that the mass spectrometer be shut down completely. When you are not using the system, place the mass spectrometer in standby mode. If you do not plan to use the system for two or more months, you can shut down the mass spectrometer completely.

#### Contents

- Shutting Down the System in an Emergency
- Opening the Tune Plus Window
- Placing the Mass Spectrometer in Standby Mode
- Turning On the Mass Spectrometer
- Shutting Down the Mass Spectrometer Completely
- Starting the System after a Complete Shutdown
- Resetting the Mass Spectrometer
- Resetting Tune and Calibration Parameters
- Restarting the Data System
- Turning Off Selected Mass Spectrometer Components

# Shutting Down the System in an Emergency



**CAUTION** If you must turn off the mass spectrometer in an emergency, **turn off the main power switch** located on the right-side power panel (Figure 9 on page 12). This switch turns off all power to the mass spectrometer, including the forepump, without harming components within the instrument. However, do not use this method as part of the standard shutdown procedure. Instead, see "Shutting Down the Mass Spectrometer Completely" on page 30.

To turn off the LC, autosampler, and data system computer in an emergency, use their respective on/off switch or button.

# **Opening the Tune Plus Window**

There are several ways to open the Tune Plus window (Figure 18).

#### ✤ To open the Tune Plus window

Do one of the following:

- On the Windows taskbar, choose Start > All Programs > Thermo Instruments > LTQ > LCQ Fleet Tune.
- In the Xcalibur<sup>™</sup> application, click the **Roadmap View** icon, the **Instrument Setup** icon, the **LCQ Fleet MS** icon, and then **Tune Plus**.

-or-

• In the Xcalibur application, click the **Roadmap View** icon (under the menu bar), the **Instrument Setup** icon, and then the **LCQ Fleet MS** icon. Then, from the main toolbar choose **LCQ Fleet > Start Tune Plus**.

Figure 18. Tune Plus window

| 🖗 Thermo Tune Plus - Untitled                             | - • •                |
|---|----------------------|
| File View Control ScanMode Display Setup Diagnostics Help |                      |
|   | <b>Q</b> FLEET       |
| ि 🗐 🌢 🕈 🕈 🔿 🔀 🔀 🗹 🛣                                       |                      |
| No spectral data available.                               |                      |
| For Help, press F1  | NUM 9/5/2014 4:38 PM |

# **Placing the Mass Spectrometer in Standby Mode**

If you are temporarily not using the LCQ Fleet MS, you do not need to shut it down completely. Instead, place the mass spectrometer in standby mode.

### **\*** To place the mass spectrometer in Standby mode

- 1. Complete all data acquisition, if any.
- 2. Open the Tune Plus window (see page 28).
- 3. If your LC/MS system includes an LC pump, turn off the liquid flow to the API source.

When controlling the LC pump through the Xcalibur data system, use the Inlet Direct Control dialog box to turn off the solvent flow. For example, to turn off the solvent flow from an Accela<sup>™</sup> pump, do the following:

- a. In the Xcalibur Instrument Setup window, click the icon for the LC pump.
- b. In the menu bar, choose **Setup > Inlet Direct Control**.
- c. Click the tab for the LC pump, and then select the **Take Pump Under Control** check box.
- d. Click the **Stop** button.

4. In the Tune Plus window, do one of the following:

• If the instrument is off, choose **Control > Standby**.

-or-



• If the instrument is on, click the **On/Standby** button to select the **Standby** mode.

This button cycles through the power modes shown in the left margin.

The LC/MS system is now in standby mode. Once the API source probe and housing have cooled to room temperature, you can safely remove these components. For instructions, refer to Chapter 2, "Setting Up the API Source," in the *LCQ Fleet Getting Started Guide*.



**CAUTION** If you are using APPI, do not leave the LC or other liquid delivery device on while the instrument is in standby mode. The absence of sheath and auxiliary gas can cause the hot vacuum ultraviolet (VUV) vacuum lamp to break upon contact with liquids.

The instrument turns off the electron multiplier, conversion dynode, 8 kV power to the API source, main rf voltage, and ion optic rf voltages. The instrument also turns off the sheath, auxiliary, and sweep gas flows.

**Note** In LTQ<sup>™</sup> version 2.7 SP1 or later, when you place the instrument in standby mode, the sweep gas flow remains on to help clean out the API source.

See Table 5 on page 36 for the on/off status of the instrument components when the instrument is in standby mode. The System LED on the front panel (Figure 8 on page 11) turns yellow when the system is in standby mode.

# **Turning On the Mass Spectrometer**

- To turn on the mass spectrometer
- 1. Open the Tune Plus window (see page 28).
- 2. Click the **On/Standby** button to select the **On** mode.



The System LED on the front panel turns green. The high voltage to the electron multiplier turns on.

# **Shutting Down the Mass Spectrometer Completely**

Shut down the LCQ Fleet MS completely only when you are not using it for an extended period of time or when you must shut it down for maintenance or service. You do not need to shut down the system completely if your work stoppage is temporary, such as overnight or through the weekend. Instead, place the system in standby mode as described in "Placing the Mass Spectrometer in Standby Mode" on page 29.



**CAUTION Hot surface.** Allow heated components to cool to room temperature (approximately 20 minutes) before servicing them.

### To shut down the mass spectrometer completely

1. Turn off the flow of sample solution from the LC (or other sample introduction device).

**Note** For instructions about operating the LC from the front panel, refer to the LC manual.

- 2. Follow the procedure, "Placing the Mass Spectrometer in Standby Mode" on page 29.
- 3. Place the electronics service switch in the Service Mode (down) position.

This turns off the power to the nonvacuum system electronics.

4. Turn off the Main Power switch.

The following occurs:

• All power to the mass spectrometer, including the turbomolecular pump and forepump, turns off. All LEDs on the front panel are off.

- After approximately 5 seconds, power to the vent valve solenoid shuts off, the vent valve opens, and the vacuum manifold vents with dry nitrogen. You can hear a hissing sound.
- After about 2 minutes, the vacuum manifold is at atmospheric pressure.
- 5. Unplug the instrument's power supply cord from the electrical outlet.



**CAUTION** Do not disconnect the power supply cord at the instrument while the other end is still plugged into the electrical outlet.

6. (Optional) Follow the next procedure, "To turn off the LC, gases, data system, and autosampler."

**Tip** If you only plan to perform routine or preventive system maintenance on the mass spectrometer, you do not need to turn off the LC, gases, data system, and autosampler. In this case, the shutdown procedure is complete. However, if you plan to have the system off for an extended period of time, Thermo Fisher Scientific recommends turning off these other parts of the LC/MS system.

### \* To turn off the LC, gases, data system, and autosampler

- 1. If the LC system is included, turn it off as described in the LC manual.
- 2. Turn off the helium and nitrogen gas supplies at their tanks.
- 3. Shut down the data system computer, and turn off the monitor and printer, as applicable.
- 4. If the autosampler is included, turn it off by using its on/off switch.

### Starting the System after a Complete Shutdown

To start the LCQ Fleet system after it has been shut down completely, follow these procedures:

- Starting the LC System
- Starting the Data System
- Starting the Mass Spectrometer
- Starting the Autosampler (as applicable)

### **Starting the LC System**

To start the LC system, follow the startup procedure described in the manufacturer's manual. If necessary, configure the LC as described in the *LCQ Fleet Getting Connected Guide*.

**IMPORTANT** To avoid wasting solvent, do not turn on the liquid flow to the mass spectrometer at this point in the procedure.

### **Starting the Data System**

### ✤ To start the data system

Turn on the computer and monitor, and, if applicable, the printer.

### **Starting the Mass Spectrometer**

Make sure that the data system is running before you start the mass spectrometer. The mass spectrometer does not operate until it receives instructions from the data system.

### To start the mass spectrometer

- 1. Turn on the flows for the helium and nitrogen gases at their tanks, if they are off.
- 2. Turn off the Main Power switch and place the electronics service switch in the Service Mode (down) position.
- 3. Plug in the power supply cord for the mass spectrometer.
- 4. Turn on the Main Power switch.

This turns on the forepump and the turbomolecular pump. All LEDs on the front panel are off.

- 5. Wait at least 1 hour to allow the mass spectrometer to pump down.
- 6. Place the electronics service switch in the Electronics Normal (up) position.

The following occurs:

- The Power LED on the front panel turns green to indicate that the electronics have power. However, the electron multiplier, conversion dynode, 8 kV power to the API source, main rf voltage, and ion optic rf voltage remain off.
- The instrument's embedded computer starts. After several seconds the Communication LED turns yellow to indicate that the data system and the instrument have started to establish a communication link.

- After several more seconds, the Communication LED turns green to indicate that the mass spectrometer and the data system are communicating. Make sure that the instrument console window is active. The data system transfers operational software to the mass spectrometer.
- After three minutes, the System LED turns yellow to indicate that the software transfer from the data system to the mass spectrometer is complete and the mass spectrometer is in standby mode. When you change the mode from standby to on, the System LED turns green to indicate that the mass spectrometer is functional and the high voltages are on.

**IMPORTANT** On the front panel, the Vacuum LED illuminates green only when the pressure in the vacuum manifold is below the maximum allowable pressure  $(5 \times 10^{-4} \text{ Torr in the analyzer region, and } 2 \text{ Torr in the ion transfer tube-skimmer region}).$ 

Although you can calibrate the mass spectrometer after the Vacuum LED turns green, you must allow the mass spectrometer's vacuum system to stabilize completely. This requires approximately 15–24 hours of continuous pumping to ensure that the calibrations are correct.

### **Starting the Autosampler**

Turn on the autosampler by using its on/off power switch. If necessary, configure the autosampler. The *LCQ Fleet Getting Connected Guide* provides procedures for connecting the mass spectrometer to the autosampler by using a contact closure cable. For procedures for placing sample vials, preparing solvent and waste containers, installing syringes, and so on, refer to the autosampler manual.

# **Resetting the Mass Spectrometer**

In the unlikely event that communication is lost between the mass spectrometer and data system computer, you can reset the instrument by using the reset button on the right-side power panel, shown in Figure 9 on page 12.

The following procedure assumes that power to the mass spectrometer and data system computer are on and that both are operational. If the mass spectrometer, data system computer, or both are off, see "Starting the System after a Complete Shutdown" on page 31.

### ✤ To reset the mass spectrometer

Hold down the reset button for 3 seconds.

The following occurs:

- The embedded computer restarts. All LEDs on the front panel turn off except the Power LED.
- After several seconds, the Communication LED turns yellow to indicate that the data system and the mass spectrometer are starting to establish a communication link.
- After several more seconds, the Communication LED turns green to indicate that the data system and the mass spectrometer are communicating. The data system transfers operational software to the instrument.
- After three minutes, the System LED turns yellow to indicate that the software transfer from the data system to the mass spectrometer is complete and the mass spectrometer is in standby mode. Or, the System LED turns green to indicate that the mass spectrometer is functional and the high voltages are on.

# **Resetting Tune and Calibration Parameters**

If you must reset the tune and calibration parameters to their factory default values, contact your local Thermo Fisher Scientific field service engineer for assistance.

### **IMPORTANT**

- Before resetting the instrument parameters to their default values, make sure that the system problems you are experiencing are not due to improper API source settings (such as spray voltage, sheath and auxiliary gas flow, or ion transfer tube temperature).
- If you reset the instrument to the factory calibration settings, always repeat the calibration of the internal electronic devices as specified in the *LCQ Fleet Getting Started Guide*. Otherwise, all instrument calibrations might produce incorrect results.

## **Restarting the Data System**

If possible, use the Windows procedure to shut down and restart the data system so that Windows can properly close applications and save changes to any open Thermo applications.

**Note** After you reset the data system, the communications link between the data system and the mass spectrometer is automatically reestablished. When this occurs, the Communication LED turns yellow and then green. If the system is unable to reestablish the communications link, hold down the reset button for three seconds.

#### To restart the data system by using Windows

- 1. On the Windows taskbar, choose **Start**, and then click the arrow next to Shut Down.
- 2. Choose Restart, and then click OK.

#### To restart the data system by using the power button

- 1. Press the power button on the data system computer.
- 2. Wait at least 20 seconds after the computer shuts down.
- 3. Press the power button again.

## **Turning Off Selected Mass Spectrometer Components**

There are five ways that you can turn off some or all of the instrument components:

- Turn off individual mass spectrometer components by using the Tune Plus window. Turning off individual components might be necessary when troubleshooting a problem or running certain diagnostic procedures.
- Place the mass spectrometer in standby mode, which is the normal state to leave the instrument in when it is not in use.
- Place the mass spectrometer in off mode, which is similar to standby, except that all high-voltage components of the instrument are off.
- Place the electronics service switch in the Service Mode (down) position so that you can perform maintenance procedures involving nonvacuum system components of the instrument.
- Turn off the Main Power switch, which removes all power to the instrument, including the vacuum system.

Table 5 summarizes the on/off status of mass spectrometer components, voltages, and gas flows.

| Mass spectrometer component                              | Standby<br>mode | Off<br>mode | Electronics<br>service switch,<br>Service Mode position | Main Power switch,<br>Off (0) position |
|--|-----------------|-------------|---|--|
| Vent valve   | Closed          | Closed      | Closed  | Open (5 sec)                           |
| APCI corona discharge needle                             |                 |             |   |  |
| APCI vaporizer   |                 |             |   |  |
| Conversion dynode  |                 |             |   |  |
| Electron multiplier                                      |                 |             |   |  |
| ESI needle   |                 |             |   |  |
| Gas, auxiliary   |                 |             |   |  |
| Gas, sheath  | Off             |             |   |  |
| Gas, sweep (LTQ version 2.7 or earlier)                  |                 |             |   |  |
| Ion optics multipoles rf voltages                        | Off             |             |   |  |
| Mass analyzer, rf/waveform voltages                      |                 |             |   |  |
| Power supply, 8 kV                                       |                 | - Chi       |   |  |
| Power supply, electron<br>multipliers/conversion dynodes |                 | Off         | Off   |  |
| API ion transfer tube dc offset                          |                 |             |   |  |
| API tube lens  |                 |             |   |  |
| Ion optics lens  |                 |             |   |  |
| Ion optics multipoles dc offset voltages                 |                 |             |   |  |
| Mass analyzer, dc offset voltage                         | On              |             |   |  |
| Power supply, 300 Vdc                                    |                 |             |   |  |
| Gas, sweep (LTQ version 2.7 SP1 or later)                |                 |             |   |  |
| API ion transfer tube heater                             |                 |             |   |  |
| Fan, rf coil   |                 |             |   |  |
| Gauge, Convectron  | On              |             |   |  |
| Gauge, ion   |                 |             |   |  |
| Power supply, PS1  |                 |             |   |  |

 Table 5.
 On/off status of mass spectrometer components, voltages, and gas flows (Sheet 1 of 2)

| Mass spectrometer component    | Standby<br>mode | Off<br>mode | Electronics<br>service switch,<br>Service Mode position | Main Power switch,<br>Off (O) position |
|--------------------------------|-----------------|-------------|---|--|
| Fan, turbomolecular pump       |                 |             |   |  |
| Fans, electronics tower        |                 |             |   |  |
| Forepump                       |                 |             |   | Off                                    |
| Power supply, PS2              | On              | On          | On  | Oli                                    |
| Turbomolecular pump            |                 |             |   |  |
| Turbomolecular pump controller |                 |             |   |  |
| Gas, helium                    |                 |             |   | On                                     |

 Table 5.
 On/off status of mass spectrometer components, voltages, and gas flows (Sheet 2 of 2)

**3** System Shutdown, Startup, and Reset Turning Off Selected Mass Spectrometer Components

# 4

# **Daily Operation**

To ensure the proper operation of the LCQ Fleet system, Thermo Fisher Scientific recommends that you perform daily preventive maintenance. This chapter specifies the items to check before operating the system and the cleaning procedures to perform after completing the analyses. You do not need to tune (that is, optimize the tune parameters for the ESI calibration solution) or calibrate the LCQ Fleet system as part of your daily routine.

Generally, 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 calibrate the LCQ Fleet system by using the ESI calibration solution about once every month. Do some calibrations, such as for the electron multiplier gain, more often. For information about tuning and calibration, refer to the *LCQ Fleet Getting Started Guide*.

**Tip** Plan to check the optimization of the tune parameters by creating a new tune method whenever you change the type of experiment, the specific compound, or the compound class.



**CAUTION** Pump down times of less than 15 hours on new instruments or after venting the mass spectrometer might cause incorrect calibration and might increase the aging of the electron multipliers.

#### Contents

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

# **Before Operating the LCQ Fleet System**

Before beginning the first analysis of the day, make sure the system is turned on (see "Turning On the Mass Spectrometer" on page 30) and follow these preventive maintenance procedures:

- Checking the Vacuum Pressure Levels
- Checking the Gas Supplies
- Checking the ESI Fused-Silica Sample Tube for Elongation

### **Checking the Vacuum Pressure Levels**

Before beginning your daily operation, check the vacuum pressure levels in the system and check for major air leaks in the system. If there is a major air leak, the system does not pump down to sufficient levels to turn on the system.



**CAUTION** For proper performance, operate the LCQ Fleet system at the proper vacuum levels. Operating the system with poor vacuum levels can cause reduced sensitivity, tuning problems, and reduced electron multiplier life.

#### ✤ To check the vacuum pressure

 In the Tune Plus window, choose Setup > Vacuum to open the Vacuum dialog box (Figure 19).





2. Check the Ion Gauge Pressure readback.

This readback displays the current pressure in the analyzer region.

3. Check the Convectron Gauge Pressure readback.

This readback displays the current pressure in the ion transfer tube–skimmer and foreline region.

4. Compare the current values of the pressures in the vacuum manifold with the following values.

| Condition  | lon gauge reading<br>(analyzer region) | Convectron gauge reading<br>(foreline, tube–skimmer region) |
|--|--|---|
| Open ion transfer tube<br>orifice, ion transfer tube at<br>250 °C (482 °F) | $0.75 - 1.5 \times 10^{-5}$ Torr       | 1.0–1.5 Torr  |

### **IMPORTANT**

- If the current values are higher than normal, there might be an air leak or the helium flow might be insufficient.
- If the pressure is above  $5 \times 10^{-5}$  Torr in the analyzer region and the system restarted within the last 30 to 60 minutes, wait another 30 minutes and recheck the pressure. If the pressure decreases with time, check the pressure periodically until it is within the typical range for the instrument.
- If the pressure remains high, the system might have an air leak.

#### To check the system for major air leaks

Listen for a rush of air or a hissing sound coming from the instrument.

Possible causes of a major leak might be a loose or disconnected fitting, an improperly positioned O-ring, or an open valve.

### ✤ To fix an air leak

- 1. Shut down the system (see "Shutting Down the Mass Spectrometer Completely" on page 30).
- 2. Visually inspect 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 and O-rings are properly positioned.

### **Checking the Gas Supplies**

Check the helium gas tank's regulator. Make sure that there is sufficient gas for the analysis, which is a minimum of 3447 kPa (500 psi) on the high pressure gauge of the regulator. If necessary, replace the tank. Verify that the pressure of helium gas reaching the mass spectrometer is 275  $\pm$ 70 kPa (40  $\pm$ 10 psi). If necessary, adjust the pressure with the tank pressure regulator.

Check the nitrogen gas supply on the regulator of the nitrogen gas tank or liquid nitrogen boil-off tank. Make sure that there is sufficient gas for the analysis. If necessary, replace the tank. Verify that the pressure of nitrogen gas reaching the instrument is 690  $\pm$ 140 kPa (100  $\pm$ 20 psi). If necessary, adjust the pressure with the tank pressure regulator.

**Note** When you operate the LCQ Fleet system 24 hours and 7 days a week, typical daily consumption of nitrogen gas is  $5560-26700 \text{ L} (196-943 \text{ ft}^3)$ .

For more information about gas requirements, refer to the *LCQ Fleet Preinstallation Requirements Guide*.

### **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, which can degrade both signal intensity and stability over time.

If you are using a fused-silica sample tube in the ESI mode, verify that the sample tube is not elongated past the tip of the ESI spray needle. If the tube is elongated, cut and reposition it. See "Trimming the ESI Sample Tube" on page 53.

# After Operating the LCO Fleet System

Follow these preventive maintenance procedures every day after operating the system:

- Flushing the Inlet Components (as needed)
- Cleaning the Ion Sweep Cone, Spray Cone, and Ion Transfer Tube
- Purging the Oil in the Forepump
- Emptying the Solvent Waste Container
- Placing the System in Standby Mode

### **Flushing the Inlet Components**

This section describes how to flush the inlet components (sample transfer line, sample tube, and API probe) at the end of each work day (or more often if you suspect they are contaminated). You use a 50:50 methanol/water solution from the LC system through the API source at a flow rate of 200–400  $\mu$ L/min for approximately 15 minutes to remove contamination.

**Tip** You do not need to flush the inlet components daily. However, if a spectrum shows unwanted contamination peaks, follow this procedure to flush the inlet components.

### To flush the inlet components

- 1. Complete all data acquisition, if any.
- 2. Open the Tune Plus window (see page 28).



- 3. Make sure that the **On/Standby** button indicates the **On** mode, and then do one of the following:
  - If operating in APCI or APPI mode, go to step 4.
  - If operating in ESI mode, go to step 5.
- 4. Flush the APCI source as follows:
  - a. Choose **Setup > APCI Source** to open the APCI Source dialog box (Figure 20).

### Figure 20. APCI Source dialog box

| APCI Source                         |        |                                       | ×      |
|-------------------------------------|--------|---------------------------------------|--------|
|                                     |        |                                       | Actual |
| ⊻aporizer Temp (°C):                | 0.00   | ÷                                     | 30.29  |
| <u>S</u> heath Gas Flow Rate (arb): | 50     | *<br>*                                | -0.01  |
| Aux <u>G</u> as Flow Rate (arb):    | 5      | · •                                   | -0.00  |
| S <u>w</u> eep Gas Flow Rate (arb): | 5      | *<br>*                                | -0.01  |
| Djscharge Current (µA):             | 5.00   | ·                                     | 0.04   |
| Discharge Voltage (kV)  :           |        |                                       | 0.01   |
| <u>C</u> apillary Temp (°C):        | 275.00 | *<br>*                                | 275.06 |
| S-Lens R <u>F</u> Level (%):        | 60.0   | · · · · · · · · · · · · · · · · · · · |        |
|                                     |        |                                       |        |
| Apply OK Ca                         | ancel  | <u>H</u> e                            | elp    |

- b. In the Vaporizer Temp (°C) box, enter **500**.
- c. In the Sheath Gas Flow Rate (arb) box, enter 30.
- d. In the Aux Gas Flow Rate (arb) box, enter 5.
- e. In the Sweep Gas Flow Rate (arb) box, enter **0**.
- f. In the Discharge Current ( $\mu A$ ) box, enter **0**.

- g. Click OK.
- h. Go to step 6.
- 5. Flush the ESI source as follows:
  - a. Choose **Setup > ESI Source** to open the ESI Source dialog box (Figure 21).

**Figure 21.** ESI Source dialog box

| ESI Source                  |        | ×            |
|-----------------------------|--------|--------------|
|                             |        | Actual       |
| Sheath Gas Flow Bate (arb): | 8      | 8.00         |
| Aux Gas Flow Bate (arb):    |        | -0.00        |
| Sween Gas Flow Bate (arb):  |        | -0.00        |
|                             | 5.00   | 4 98         |
| Sprau Current (uA):         | 0.00   | 2.45         |
| Capillaru Temp (*C):        | 275.00 | 275.03       |
| S.J. and BE Level (%):      | E4.5   | 210.00       |
|                             | 04.3   |              |
|                             | Cancel | <u>H</u> elp |

- b. In the Sheath Gas Flow Rate (arb) box, enter 30.
- c. In the Aux Gas Flow Rate (arb) box, enter 5.
- d. In the Sweep Gas Flow Rate (arb) box, enter 0.
- e. In the Spray Voltage (kV) box, enter 0.
- f. Click OK.
- 6. Set up and start a flow of 50:50 methanol/water solution from the LC system to the API source as follows:
  - a. Choose Setup > Inlet Direct Control to open the Inlet Direct Control dialog box.

The Xcalibur data system controls the LC pumps from several manufacturers including Thermo Fisher Scientific, Agilent<sup>™</sup> Technologies, and Waters<sup>™</sup> Corporation. Contact your Thermo Fisher Scientific sales representative for information about the liquid chromatography systems compatible with the LCQ Fleet MS.

- b. Click the **LC Pump** tab.
- c. Set the solvent proportions to 50% methanol and 50% water.
- d. Start the solvent flow.
- 7. Let the solution flow through the sample transfer line, sample tube, and API probe for 15 minutes.

- 8. 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 the **Pump Off** or **Stop Pump** button.
- 9. After another 5 minutes, click the **On/Standby** button to select the **Standby** mode.

### **Cleaning the Ion Sweep Cone, Spray Cone, and Ion Transfer Tube**

Clean the ion sweep cone, spray cone, and ion transfer tube on a regular basis to prevent corrosion and to maintain optimum performance of the API source. A good practice is to wash or flush the ion sweep cone and ion transfer tube at the end of each operating day after you pump a solution of 50:50 methanol/water from the LC system through the sample transfer line, sample tube, and API probe (see "Flushing the Inlet Components" on page 43). If you use a mobile phase that contains a nonvolatile buffer or inject high concentrations of sample, you might need to clean these parts more often. It is not necessary to vent the system to flush the ion sweep cone and ion transfer tube.



**CAUTION** When the ion transfer tube is installed, do not flush it with cleaning solution, which flushes the residue into the mass spectrometer.

For detailed cleaning instructions, refer to Chapter 8 in the LCQ Fleet Getting Started Guide.

### **Purging the Oil in the Forepump**

Purge (decontaminate) the oil in the forepump daily to remove water and other dissolved chemicals, which 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 tube. For instructions, refer to the forepump's documentation.

**IMPORTANT** Remember to close the purge valve before continuing normal operation.

### **Emptying the Solvent Waste Container**

Check the solvent level in the solvent waste container daily. If necessary, empty the container and dispose of the solvent waste in accordance with local and national regulations.

### Placing the System in Standby Mode

After you complete the daily maintenance procedures, place the instrument in standby mode as described in "Placing the Mass Spectrometer in Standby Mode" on page 29.



4 Daily Operation After Operating the LCQ Fleet System

# 5

# Maintenance

This chapter provides routine maintenance procedures that you must perform to ensure optimum performance of the LCQ Fleet mass spectrometer. Optimum performance depends on the maintenance of all parts of the instrument. You are responsible for maintaining the system properly by performing the system maintenance procedures on a regular basis.

For a list of replaceable parts, see Chapter 7, "Replaceable Parts."

### Contents

- Maintenance Schedule
- Tools and Supplies
- Guidelines
- Maintaining the API Source Housing
- Maintaining the API Source Probe
- Maintaining the API Source Interface
- Maintaining the Q00-L0 RF Lens
- Maintaining the Q0 and Q1 Ion Optics
- Replacing the Electron Multiplier
- Maintaining the Forepump
- Maintaining the Fan Filter

# **Maintenance Schedule**

Table 6 lists the maintenance procedures, their recommended frequency, and their location in this guide.

| requency |
|----------|
| ľ        |

| Component  | Procedure   | Frequency   | Location                      |
|--|---|---|-------------------------------|
| API source   | Flush (clean) the sample transfer<br>line, sample tube, and API probe.  | Daily   | page 43<br>page 53<br>page 65 |
|  | Clean the API source housing.   | As needed   | page 51                       |
|  | Trim the sample tube.   | If the polyimide coating on the end<br>of the sample tube is elongated    | page 53                       |
|  | Replace the sample tube and safety sleeve.                              | If the sample tube is broken or obstructed                                | page 59                       |
| API source interface                                     | Clean the ion sweep cone and spray cone.                                | Daily or more often depending on analytical conditions                    |                               |
|  | Remove and clean the ion transfer tube.                                 | Weekly, or if the ion transfer tube<br>bore is contaminated or obstructed | -                             |
|  | Replace the ion transfer tube.  | If the bore becomes corroded or blocked                                   | page 73                       |
|  | Clean the skimmer and tube lens.  | As needed, depending on analytical conditions                             | -                             |
|  | Clean the exit lens or S-lens.  | As needed, depending on analytical conditions                             | -                             |
| Q00 rf lens, and<br>lens L0                              | Clean multipole Q00 and lens L0.  | As needed, depending on analytical conditions                             | page 83                       |
| Q0 and Q1 ion optics,<br>lens L1, and<br>split gate lens | Clean multipole Q0 and Q1 ion optics, lens L1, and the split gate lens. | As needed, depending on analytical conditions                             | page 89                       |
| Forepump   | Purge (decontaminate) the oil and check for leaks.                      | Daily   | page 104                      |
|  | Add oil.  | As needed, based on oil level   | - Also, refer to the pump's   |
|  | Change the oil.   | Every 3 months, or if the oil is cloudy or discolored                     | documentation.                |
| Cooling fans   | Clean the air filter.   | Every 4 months  | page 104                      |

For instructions about maintaining the LC modules, refer to that instrument's manual.

# **Tools and Supplies**

The LCQ Fleet MS requires very few tools to perform routine maintenance procedures. You can remove and disassemble many of the components by hand. Table 7 lists the necessary chemicals, tools, and equipment for maintaining the instrument. (Two of the tools are already in the kits.) In addition, you can use the contents of the Preventive Maintenance (PM) Cleaning Kit (P/N 97455-62051).



### CAUTION Avoid exposure to potentially harmful materials.

By law, producers and suppliers of chemical compounds are required to provide their customers with the most current health and safety information in the form of Material Safety Data Sheets (MSDSs) or Safety Data Sheets (SDSs). The MSDSs and SDSs must be freely available to lab personnel to examine at any time. These data sheets describe the chemicals and summarize information on the hazard and toxicity of specific chemical compounds. They also provide information on the proper handling of compounds, first aid for accidental exposure, and procedures to remedy spills or leaks.

Read the MSDS or SDS for each chemical you use. Store and handle all chemicals in accordance with standard safety procedures. Always wear protective gloves and safety glasses when you use solvents or corrosives. Also, contain waste streams, use proper ventilation, and dispose of all laboratory reagents according to the directions in the MSDS or SDS.

| Description                               | Part number  |
|---|--|
| Chemicals                                 |  |
| Acetone (or other suitable polar solvent) |  |
| HPLC grade                                | Fisher Scientific <sup>™</sup> A949  |
| GC Resolv™                                | Fisher Scientific A928-4<br>(amber glass, 4 L)                                     |
| Detergent (for example, Liquinox™)        | (Liquinox) Fisher Scientific:<br>• 50-821-299 (1 quart)<br>• 50-821-298 (1 gallon) |
| Methanol, LC/MS-grade                     | Fisher Scientific A456-1   |
| Nitrogen gas, clean and dry               | -  |
| Water, LC/MS-grade                        | Fisher Scientific W6-1   |
| Water, tap                                | -  |

**Table 7.** Chemicals, tools, and equipment (Sheet 1 of 2)

| Description   | Part number  |
|---|--|
| Tools   |  |
| Fused-silica cutting tool   | _  |
| Hex ball driver, 3 mm   | 00725-00048 <sup>a</sup>   |
| Hex driver (or ball driver), 1/4 in.  | -  |
| Hex ball driver set: 0.050 in., 1/16 in., 5/64 in., 3/32 in., 7/64 in., 1/8 in., 9/64 in., 5/32 in., and 3/16 in.   | 00025-03025  |
| Ion transfer tube removal tool  | 70111-20258 <sup>b</sup>   |
| Screwdriver, Phillips #2  | _  |
| Screwdrivers, slotted: large and small  | _  |
| Wrenches, open-end: 5/16 in., 3/8 in., and 1/2 in.  | _  |
| (Optional) Toothbrush, soft (or similar tool)   | -  |
| (Optional) Tweezers, plastic (or similar tool)  | -  |
| Equipment   |  |
| Aluminum foil, heavy gauge <sup>c</sup>   | Fisher Scientific 01-213-104   |
| Beaker or graduated cylinder (for use with methanol)  | -  |
| Chamois-tipped swabs  | 00301-01912  |
| Gloves, lint-free and powder-free   | Fisher Scientific 19-120-2947 <sup>d</sup>                                     |
|   | Unity Lab Services:<br>• 23827-0008 (size medium)<br>• 23827-0009 (size large) |
| Industrial tissues, lint-free   | -  |
| Magnification device  | -  |
| MICRO-MESH <sup>™</sup> polishing swabs, 6000 grit (light purple color), 2.25 in. long <sup>e</sup>   | 00301-01911  |
| Sonicator   | -  |
| <ul> <li><sup>a</sup> Provided in the HESI-II Probe Kit</li> <li><sup>b</sup> Provided in the MS Accessory Kit</li> <li><sup>c</sup> Rinse each sheet with acetone before use.</li> </ul> |  |

### **Table 7.** Chemicals, tools, and equipment (Sheet 2 of 2)

<sup>d</sup> Multiple sizes are available.

<sup>e</sup> Provided in the optional PM Cleaning Kit

## Guidelines

For optimal results, follow these guidelines when performing the procedures in this chapter:

- Always wear a new pair of lint- and powder-free gloves when handling internal components. Never reuse gloves after you remove them because the surface contaminants on them recontaminate clean parts.
- Always place the components on a clean, lint-free work surface.
- Have nearby the necessary tools, supplies, and replacement parts (when applicable).
- Never overtighten a screw or use excessive force.
- Proceed methodically.

### IMPORTANT

- Put on a new pair of lint- and powder-free gloves before starting each removal, cleaning, and reinstallation procedure.
- Make sure that you do not introduce any scratches or surface abrasions while handling the API source interface components. Even small scratches can affect performance if they are close to the ion transmission path. Avoid using tools, such as metal pliers, that might scratch these components.

# **Maintaining the API Source Housing**

Only Thermo Fisher Scientific field service engineers can service the API source housing, while user maintenance is limited to cleaning the housing as necessary. Follow all safety precautions in the *Ion Max and Ion Max-S API Source Hardware Manual* regarding the installation and removal of the API source. For any additional service, contact your local Thermo Fisher Scientific field service engineer.

### To clean the API source housing

- 1. Remove the Ion Max<sup>™</sup> or Ion Max-S API source housing from the mass spectrometer.
- 2. In an appropriate fume hood, rinse the interior of the housing with LC/MS-grade methanol.
- 3. Allow the housing to dry before you install it on the mass spectrometer.

# **Maintaining the API Source Probe**

This section contains information for maintaining the API source probes:

- ESI Probe Maintenance
- HESI-II Probe Maintenance
- APCI Probe Maintenance

For API source probe maintenance tasks, you need the following tools and supplies (see also Table 7 on page 49).

| Tools                     | Supplies                          |
|---------------------------|-----------------------------------|
| Fused-silica cutting tool | Chamois-tipped swabs              |
| Magnification device      | Gloves, lint-free and powder-free |
| 7/64 in. hex driver       | Lint-free industrial tissues      |
| 5/16 in. open-end wrench  | Methanol, LC/MS-grade             |
| 3/8 in. open-end wrench   | Nitrogen gas                      |
| 1/2 in. open-end wrench   | Water, LC/MS-grade                |

#### **IMPORTANT**

- Prepare a clean work surface by covering the area with lint-free paper.
- Put on a new pair of lint- and powder-free gloves before starting each of these removal, cleaning, and reinstallation procedures.

### **ESI Probe Maintenance**

The ESI probe requires minimum maintenance. If the fused-silica sample tube is plugged or broken, replace it. You can trim or replace the sample tube without disassembling the ESI probe. However, to clean the nozzle bore or the interior surfaces of the ESI manifold or to replace the electrospray needle or needle seal, you must disassemble the ESI probe.



**CAUTION Hot surface.** At operating temperatures above 350 °C (662 °F), the probe and API source housing can severely burn you.

- Before removing the probe or API source housing, allow the part to cool to room temperature (approximately 20 minutes) before touching it.
- If the instrument connects to an LC system, leave the solvent flow from the LC pump on while the probe cools to room temperature.

### To maintain the ESI probe, follow these procedures:

- Flushing the Sample Transfer Line and Sample Tube
- Trimming the ESI Sample Tube
- Disassembling the ESI Probe
- Cleaning or Replacing the ESI Probe Components
- Assembling the ESI Probe
- Installing a Fused-Silica Sample Tube and PEEK Safety Sleeve
- Installing an Optional Metal Sample Tube

### Flushing the Sample Transfer Line and Sample Tube

You can minimize cleaning of the probe components by flushing the sample transfer line, sample tube, and probe at the end of each work day (or more often if you suspect they are contaminated). To remove contamination, use a 50:50 solution of LC/MS-grade methanol and LC/MS-grade water, and flush the solution from the LC system through the API source for approximately 15 minutes. For instructions, see "Flushing the Inlet Components" on page 43.

### **Trimming the ESI Sample Tube**

Operating the instrument with acetonitrile in the mobile phase can cause elongation of the polyimide coating on the fused-silica sample tube. If the polyimide coating has elongated past the end of the electrospray needle, cut and reposition the end of the sample tube.

### \* To cut and reposition the end of the sample tube

- 1. Place the instrument in Standby mode (see page 29) and let it cool to room temperature. See the temperature cautionary statement on page 52.
- 2. Remove the ESI probe from the API source housing.

For instructions, refer to Chapter 2, "Setting Up the API Source," in the *LCQ Fleet Getting Started Guide*.

3. Loosen the red fitting of the two-piece fingertight fitting that secures the position of the sample tube and the safety sleeve at the ESI probe sample inlet (Figure 22).

**Note** When the nut and ferrule assembly are properly positioned in the receiving port, the receiving port compresses the ferrule so that it fits snugly to the tubing. When you loosen the fitting, the receiving port does not compress the ferrule and the tubing is free to move.



### Figure 22. Two-piece fingertight fitting and loosened sample inlet adapter fitting

- 4. Gently pull back on the sample tube to free it from the ferrule.
- 5. Push the sample tube forward so that it extends beyond the end of the electrospray needle.
- 6. Using the fused-silica cutting tool, cut a small length (4–5 mm) of sample tubing and then under magnification check that the end is squarely cut.
- 7. Pull the sample tube backwards until the exit end of the sample tube is flush with the ESI needle.

The optimal sample tube protrusion depends on the solvent flow rate, as follows:

- For flow rates less than or equal to 100  $\mu L/min,$  set the sample tube protrusion to 1 mm past the ESI needle tip.
- For flow rates greater than 100  $\mu$ L/min, make sure that the sample tube is flush with the ESI needle tip or recessed inside the ESI needle by less than 1 mm.
- 8. Tighten the two-piece fingertight fitting securely to hold the sample tube in place.
- 9. Because the sample tube can move forward when tightening the two-piece fingertight fitting, make sure that the sample tube is still set to the appropriate protrusion. If necessary, loosen the fitting and reposition the sample tube.
- 10. Reinstall the ESI probe into the API source housing.

### **Disassembling the ESI Probe**

To replace or clean the ESI probe components, disassemble the ESI probe.

#### To disassemble the ESI probe

- 1. Place the instrument in Standby mode (see page 29) and let it cool to room temperature.
- 2. Remove the ESI probe from the API source housing.

For instructions, refer to Chapter 2, "Setting Up the API Source," in the *LCQ Fleet Getting Started Guide*.

3. Unscrew the red fitting of the two-piece fingertight fitting from the sample inlet adapter fitting and remove the sample tube from the ESI probe.
- 4. Because the ESI manifold contains loose components (battery contact and resistor subassembly), hold the ESI probe with the nozzle facing upward.
- 5. Using the 5/16 in. open-end wrench, remove the ESI nozzle from the ESI manifold (see Figure 25 on page 58).
- 6. If the nozzle requires cleaning, follow the procedure "To clean the ESI probe nozzle" on page 56.
- 7. Pull the ESI needle out of the ESI manifold (Figure 23).

Resistor High-voltage socket High-voltage socket Sample inlet adapter fitting Sheath liquid inlet fitting ESI Needle ESI needle seal manifold

Figure 23. ESI probe with the nozzle removed

8. To dislodge the needle seal, gently tap the ESI manifold against a hard surface.

If necessary, use the needle or another appropriate tool to push the needle seal out of the ESI manifold. Tapping the manifold against a hard surface can also dislodge the resistor and battery contact.

- 9. Using the 1/2 in. open-end wrench, disconnect the high-voltage (HV) socket from the ESI probe.
- 10. Unscrew the fitting from the sheath liquid inlet.
- 11. If the ESI manifold needs cleaning, follow the procedure "To clean and dry the ESI probe manifold" on page 57.
- 12. To reassemble the ESI probe, see "Assembling the ESI Probe" on page 58.

## **Cleaning or Replacing the ESI Probe Components**

Maintaining the ESI probe requires occasional replacement of the 26-gauge needle, the needle seal, the ESI nozzle, and the HV socket O-rings. In addition, the ESI nozzle and manifold occasionally require cleaning.

| For field service use only              | Part number |
|---|-------------|
| ESI 26-gauge spray needle               | 00950-00990 |
| ESI needle seal                         | 00950-00952 |
| ESI nozzle O-ring, Viton™, 0.676 in. ID | 00107-05710 |
| ESI high-voltage socket O-ring          | 00107-02550 |

### \* To clean the ESI probe nozzle

**IMPORTANT** Always use LC/MS-grade methanol (see Table 7 on page 49).

- 1. Disconnect the ESI nozzle from the ESI manifold (see steps 3–5 in "To disassemble the ESI probe" on page 54).
- 2. Clean the bore of the ESI nozzle with methanol.

The choice of solvent depends on the solubility of the chemical deposits.

- 3. Rinse the nozzle with methanol.
- 4. Dry the component with nitrogen gas to make sure that all the solvent evaporates.
- 5. Inspect the ESI nozzle O-ring and replace it if necessary (Figure 24).

Figure 24. ESI nozzle and O-ring



6. Reconnect the ESI nozzle to the ESI manifold (see page 58).

If the needle is damaged, replace it. If the sheath gas is leaking at the interface between the needle seal and the needle, replace the needle seal.

### \* To replace the needle, needle seal, or both

- 1. Disconnect the ESI nozzle from the ESI manifold (see steps 3–5 in "To disassemble the ESI probe" on page 54).
- 2. Pull the ESI needle out of the ESI manifold.
- 3. To dislodge the needle seal, gently tap the ESI manifold against a hard surface.

If necessary, use the needle or another appropriate tool to push the needle seal out of the ESI manifold. Tapping the manifold against a hard surface can also help to dislodge the resistor and battery contact.

- 4. If necessary, replace the needle seal, the 26-gauge spray needle, or both.
- 5. Reassemble the ESI probe (see steps 1–6 in "To assemble the ESI probe" on page 58).

### \* To clean and dry the ESI probe manifold

**IMPORTANT** Always use LC/MS-grade methanol and LC/MS-grade water (see Table 7 on page 49).

- 1. Disassemble the ESI probe (see steps 3–5 in "To disassemble the ESI probe" on page 54).
- 2. Rinse the ESI manifold (Figure 25) with water and then with methanol.
- 3. Remove excess methanol from the manifold with a lint-free tissue.
- 4. Dry the component with nitrogen gas to make sure that all the solvent evaporates.
- 5. Inspect the spray needle, nozzle O-ring, HV socket O-ring, and needle seal.
- 6. Replace any damaged parts.
- 7. Reassemble the ESI probe (see the following procedure).

# **Assembling the ESI Probe**

Follow this procedure after cleaning or replacing ESI probe components.

## $\label{eq:constraint} \bullet \quad \mbox{To assemble the ESI probe}$

1. Insert the resistor and battery contact subassembly into the ESI manifold.

Figure 25. Front end of the ESI probe (exploded view)



- 2. Insert the entrance end of the ESI needle into the needle seal.
- 3. Position the ESI needle and needle seal in the ESI manifold.
- 4. Make sure that the 0.676 in. ID O-ring is in the precut groove on the ESI nozzle (Figure 24 on page 56).
- 5. Thread the ESI nozzle over the needle and into the ESI manifold. Slightly wet the nozzle threads with LC/MS-grade methanol for lubrication.
- 6. Using the 5/16 in. open-end wrench, tighten the ESI nozzle until it is a little more than fingertight—do not overtighten the nozzle.
- 7. Insert the HV socket into the back of the ESI manifold, and use the 1/2 in. open-end wrench to tighten the socket.
- 8. Reconnect the sheath liquid inlet fitting.
- 9. Install a new sample tube (see page 60).

### Installing a Fused-Silica Sample Tube and PEEK Safety Sleeve

When you use a fused-silica sample tube with the ESI or HESI-II probe, cover the exposed portion of the sample tube with a PEEK safety sleeve.



**CAUTION Avoid electrical shock.** Cover the fused-silica sample tube with the PEEK safety sleeve and use the associated PEEK ferrules provided in the Safety Sleeve Kit before operating the instrument. The PEEK tubing acts as a second level of protection against accidental electrical discharge.

Table 8 lists the parts for installing a fused-silica sample tube with the PEEK safety sleeve.

| Image | Description   | Part number |
|-------|---|-------------|
|       | Ferrule, natural PEEK, 0.027 in. ID<br>(for use with the 0.024 in. OD PEEK safety sleeve)   | 00101-18119 |
|       | Fitting, adapter, natural PEEK,10-32 to 1/4-28,<br>0.040 in. (1.0 mm) thru-hole<br>(for the ESI probe sample inlet)<br>(Upchurch Scientific <sup>™</sup> P-669) | 00101-18080 |
|       | Fitting, fingertight, natural PEEK, two wings<br>(for the 1/16 in. OD high-pressure tubing)<br>(Upchurch Scientific F-300)                                      | 00101-18081 |
|       | Fitting, fingertight, red, one wing<br>(for the 1/16 in. OD high-pressure tubing)<br>(Upchurch Scientific F-200)  | 00101-18195 |
|       | Fitting, grounding union, stainless steel,<br>0.010 in. thru-hole<br>(Upchurch Scientific U-435)  | 00101-18182 |
| _     | Safety sleeve, natural PEEK tubing,<br>230 μm ID, 610 μm OD, 25.4 cm long<br>(0.009 in. ID, 0.024 in. OD, 10 in. long)  | 00301-22806 |
| -     | Tubing, fused-silica, 100 μm ID, 193 μm OD<br>(0.003 in. ID, 0.008 in. OD)  | 00106-10499 |
| -     | Tubing, red PEEK, 127 μm ID, 1/16 in. OD<br>(0.005 in. ID, 1.6 mm OD)   | 00301-22912 |

**Table 8.** Parts for a fused-silica sample tube

To install the fused-silica sample tube, thread the sample tube through the ESI needle that protrudes from the ESI probe nozzle and the safety sleeve. Because you must thread the tubing through these small orifices, you might find a magnifying device useful.

### ✤ To install the new sample tube and PEEK safety sleeve

1. Using the fused-silica cutting tool, cut approximately 38 cm (15 in.) of fused-silica tubing, and then under magnification check that the end is cut squarely.

The piece of sample tubing must be long enough to extend through the ESI probe and the natural PEEK safety sleeve.

- 2. Remove the sample inlet adapter from the ESI probe sample inlet.
- 3. Insert the sample tube through the ESI needle that protrudes from the front of the ESI nozzle, and then push it through the ESI probe until approximately 3.5 cm (1.5 in.) protrudes past the front of the probe.

The remaining length of the sample tube protrudes from the ESI probe sample inlet at the back of the probe (Figure 26).



**Figure 26.** Fused-silica sample tube inserted through the front of the ESI probe

4. Slide the safety sleeve over the end of the sample tube that protrudes at the back of the probe sample inlet, and then push the safety sleeve into the probe until it meets resistance (Figure 27).



**CAUTION Avoid electrical shock.** You must install the PEEK safety sleeve, which acts as a second level of protection against accidental electrical discharge.



Figure 27. Natural PEEK safety sleeve installed in the sample inlet (ESI probe)

5. With the external threads facing the ESI probe sample inlet, slide the natural PEEK fitting adapter over the safety sleeve, and then fingertighten the fitting into the ESI probe sample inlet (Figure 28).





- 6. Slide the other fingertight fittings onto the PEEK sleeve (Figure 29) as follows:
  - a. Slide the natural PEEK ferrule with the tapered end facing the sample inlet onto the safety sleeve.
  - b. Slide the red, one-wing fingertight fitting with the threaded end facing the sample inlet onto the safety sleeve.
  - c. Slide the natural PEEK, two-wing fingertight fitting with the threaded end facing away from the sample inlet onto the safety sleeve.

d. Slide the natural PEEK ferrule with the tapered end facing away from the sample inlet onto the safety sleeve.



**Figure 29.** Fingertight fittings installed over the safety sleeve (ESI probe)

- 7. Connect the safety sleeve and sample tube assembly to the grounding union as follows:
  - a. Adjust the position of the sample tube so that it is flush with the end of the safety sleeve that protrudes from the back of the probe.
  - b. To provide leverage when tightening the fitting to the union, position the grounding union in the grounding union bar of the API source housing (Figure 30).

Figure 30. Grounding union positioned in the grounding bar



c. To prevent the sample tube from slipping through the grounding union thru-hole and out the other end, connect a fingertight fitting and red PEEK tubing to the other end of the grounding union. d. While holding the safety sleeve and sample tube firmly against the grounding union receiving port, manually tighten the fitting as tight as you can (Figure 31 and Figure 32).

Figure 31. Safety sleeve connection to the grounding union (ESI probe)



e. Make sure that the sample tube is held tightly in the grounded union by gently pulling it from the exit end of the ESI needle (Figure 32).





- 8. Adjust the position of the sample tube as follows:
  - a. Using the fused-silica cutting tool, cut the sample tube approximately 2.5 cm (1 in.) past the tip of the ESI needle.
  - b. From the ESI sample inlet, loosen the red PEEK fitting, and then pull the safety sleeve backwards so that the sample tube is positioned appropriately within the ESI needle (Figure 33).

The optimal position of the sample tube depends on the solvent flow rate, as follows:

- For flow rates less than or equal to 100  $\mu L/min$ , set the sample tube protrusion to 1 mm past the ESI needle tip.
- For flow rates greater than 100  $\mu$ L/min, make sure that the sample tube is flush with the ESI needle tip or recessed inside the ESI needle by less than 1 mm (Figure 34).



Figure 33. Adjusting the sample tube position (ESI probe)

- c. Tighten the fingertight fitting to secure the safety sleeve and sample tube.
- d. Because the sample tube can move forward when tightening the sample inlet fitting, make sure that the sample tube is initially recessed within the ESI needle. If necessary, loosen the red PEEK fitting and reposition the sample tube.





### Installing an Optional Metal Sample Tube

You can configure the ESI probe to use a stainless-steel metal sample tube rather than a fused-silica sample tube. Two kits are available, one that includes a 32-gauge metal sample tube for typical flow rates used in ESI and another with a 34-gauge metal sample tube used for low-flow applications. Both kits include instructions for installing the stainless steel sample tube. For part numbers, see "API Source Probes and Parts" on page 112.

## **HESI-II Probe Maintenance**

The HESI-II probe requires minimum maintenance. If the metal sample tube is plugged, replace it. Replacing the metal sample tube requires a partial disassembly of the probe.



**CAUTION Hot surface.** At operating temperatures above 350 °C (662 °F), the probe and API source housing can severely burn you.

- Before removing the probe or API source housing, allow the part to cool to room temperature (approximately 20 minutes) before touching it.
- If the instrument connects to an LC system, leave the solvent flow from the LC pump on while the probe cools to room temperature.

To maintain the HESI-II probe, follow these procedures:

- Flushing the Sample Transfer Line and Sample Tube
- Replacing the Needle Insert

#### Flushing the Sample Transfer Line and Sample Tube

You can minimize cleaning of the probe components by flushing the sample transfer line, sample tube, and probe at the end of each work day (or more often if you suspect they are contaminated). To remove contamination, use a 50:50 solution of LC/MS-grade methanol and LC/MS-grade water, and flush the solution from the LC system through the API source for approximately 15 minutes. For instructions, see "Flushing the Inlet Components" on page 43.

#### **Replacing the Needle Insert**

If the metal sample tube is plugged, you can replace the needle insert. The needle insert is assembled at the factory and consists of an adjustable union, needle guide fitting, ferrule, O-ring, ESI needle, and metal sample tube (Figure 35). The ferrule is swaged onto the ESI needle. Factory adjusted, the metal sample tube protrudes 0.5 mm from the end of the ESI needle (Figure 36).

To support flow rates of  $5-2000 \ \mu L/min$ , Thermo Fisher Scientific provides two metal needle inserts for the HESI-II probe. The difference between the two inserts is the size of the metal needle and supporting ferrule. For part numbers, see "API Source Probes and Parts" on page 112.



| For field service use only                          | Part number   |
|---|---------------|
| HESI-II probe, 32-gauge and 34-gauge needle inserts | See page 112. |

#### To replace the metal needle insert

- 1. Place the instrument in Standby mode (see page 29) and let it cool to room temperature.
- 2. Remove the HESI-II probe from the API source housing.

For instructions, refer to Chapter 2, "Setting Up the API Source," in the *LCQ Fleet Getting Started Guide*.

- 3. Unscrew the fingertight fitting from the sample inlet port.
- 4. Remove the metal needle insert from the probe as follows (Figure 37):
  - a. Using the 3 mm hex driver, remove the two M4  $\times$  35 mm long hex socket-head screws.
  - b. Pull the end cover off of the probe.
  - c. Unscrew the metal needle insert, and then pull it out of the probe body.



Figure 37. HESI-II probe disassembled (exploded view)

- 5. Insert a new metal needle insert into the probe body.
- 6. Hand-tighten the adjustable union fitting until the tip of the needle insert protrudes past the probe nozzle by 1.5 mm (Figure 38).

Figure 38. HESI-II probe nozzle tip (enlarged)



7. Place the end cover on the probe body, insert the two hex socket-head screws into the end cover, and then tighten them by using the 3 mm hex driver.

# **APCI Probe Maintenance**

The APCI probe requires minimum maintenance. Occasionally, you must clean the APCI nozzle and replace the internal APCI sample tube. The fused-silica tubing measures 150  $\mu$ m (0.006 in.) ID, 390  $\mu$ m (0.015 in.) OD, and 8.6 cm (3.4 in.) long.



**CAUTION Hot surface.** At operating temperatures above 350 °C (662 °F), the probe and API source housing can severely burn you.

- Before removing the probe or API source housing, allow the part to cool to room temperature (approximately 20 minutes) before touching it.
- If the instrument connects to an LC system, leave the solvent flow from the LC pump on while the probe cools to room temperature.

Figure 39 and Figure 40 show the major components of the APCI probe.





### To maintain the APCI probe, follow these procedures:

- 1. Flushing the Sample Transfer Line and Sample Tube
- 2. Removing the APCI Nozzle
- 3. Cleaning the APCI Nozzle
- 4. Removing the APCI Sample Tube
- 5. Installing the New APCI Sample Tube
- 6. Reassembling the APCI Probe

### Flushing the Sample Transfer Line and Sample Tube

You can minimize cleaning of the probe components by flushing the sample transfer line, sample tube, and probe at the end of each work day (or more often if you suspect they are contaminated). To remove contamination, use a 50:50 solution of LC/MS-grade methanol and LC/MS-grade water, and flush the solution from the LC system through the API source for approximately 15 minutes. For instructions, see "Flushing the Inlet Components" on page 43.

### **Removing the APCI Nozzle**

### \* To remove the APCI nozzle from the APCI probe

- 1. Place the instrument in Standby mode (see page 29) and let it cool to room temperature. See the temperature cautionary statement on page 68.
- 2. Hold the APCI probe body with one hand and with the other hand grasp the head of the APCI nozzle assembly and rotate it counterclockwise until the flat sides of the head align with the retention flanges (Figure 41).

Figure 41. Sample inlet end of the APCI probe showing locked and unlocked nozzles



3. Carefully pull out the nozzle assembly.

**CAUTION** If the sample tube hits the sides of the vaporizer, it can break. To prevent breakage, carefully pull the APCI nozzle straight back from the APCI probe.

4. Place the nozzle assembly on the clean, lint-free work surface.

## **Cleaning the APCI Nozzle**

| For field service use only                     | Part number |
|--|-------------|
| O-ring, silicone, 0.312 in. ID, 1/16 in. thick | 00107-04500 |
| O-ring, Viton, 0.500 in. ID, 1/16 in. thick    | 00107-05600 |

### \* To clean the APCI nozzle

**IMPORTANT** Always use LC/MS-grade methanol and LC/MS-grade water (see Table 7 on page 49).

- 1. Follow the procedure in "Removing the APCI Nozzle."
- 2. Check the condition of the O-rings on the APCI nozzle (Figure 42).

**Figure 42.** APCI probe nozzle assembly



- 3. Clean the interior APCI components (excluding the ceramic heater) with a 50:50 solution of methanol/water and a lint-free swab.
- 4. Dry the components with nitrogen gas to make sure that all the solvent evaporates.
- 5. Reinstall any O-rings removed while cleaning.
- 6. Do one of the following:
  - If you do not want to replace the APCI sample tube, follow the procedure "To reassemble the APCI probe" on page 73.
  - If you want to replace the sample tube, follow the procedure "To remove the APCI sample tube" on page 71.

### **Removing the APCI Sample Tube**

### ✤ To remove the APCI sample tube

- 1. Remove the APCI nozzle from the APCI probe (see page 69).
- 2. Using the 3/8 in. open-end wrench, loosen the APCI flange fitting, and then pull the sample inlet fitting, exit nut, ferrule, and sample tube assembly from the APCI nozzle (Figure 43).





3. Remove the sample tube, nut, and ferrule assembly from the APCI flange fitting (Figure 44).





4. Discard the used sample tube.

## Installing the New APCI Sample Tube

| For field service use only                  | Part number |
|---|-------------|
| O-ring, Viton, 0.239 in. ID, 1/16 in. thick | 00107-04000 |

#### ✤ To install a new APCI sample tube

- 1. Remove the APCI sample tube from the APCI nozzle (see page 71).
- 2. Check the condition of the O-ring on the APCI flange fitting (Figure 45), and replace it if necessary.
- 3. Using the fused-silica cutting tool, cut approximately 13 cm (5 in.) of fused-silica tubing, and then under magnification check that the end is cut squarely.
- 4. Connect the sample tubing to the APCI flange fitting as follows:
  - a. Slide the nut and then the ferrule onto the sample tubing (Figure 45).

Figure 45. Sample tubing connection to the APCI flange fitting



- b. While pressing the sample tubing into the externally threaded end of the APCI flange fitting, fingertighten the nut and fitting.
- 5. Carefully insert the free end of the sample tubing into the back of the APCI nozzle and out the nozzle tip, and then fingertighten the APCI flange fitting.
- 6. Using the 3/8 in. open-end wrench, tighten the APCI flange fitting an additional quarter turn (Figure 43 on page 71).
- 7. Using the fused-silica cutting tool, cut the sample tube approximately 1 mm past the tip of the APCI nozzle (Figure 46).

Figure 46. Sample tube extending past the APCI nozzle tip



## **Reassembling the APCI Probe**

### \* To reassemble the APCI probe

- 1. Hold the APCI probe body with one hand and with the other hand carefully insert the APCI nozzle into the APCI probe.
- 2. Align the flat sides of the APCI nozzle head with the retention flanges on the probe body ("unlocked nozzle" in Figure 41 on page 69).
- 3. Rotate the head of the nozzle 90 degrees clockwise to secure the rounded sides of the nozzle head under the retention flanges ("locked nozzle" in Figure 41 on page 69).

# **Maintaining the API Source Interface**

To maintain the API source interface, follow these procedures:

- Removing the API Source Interface
- Cleaning the Skimmer and Tube Lens
- Cleaning the API Ion Transfer Tube, Spray Cone, and Ion Sweep Cone
- Reinstalling the API Source Interface

For API source interface maintenance tasks, you need the following tools and supplies (see also Table 7 on page 49).

| Tools  | Supplies                             |
|--|--------------------------------------|
| Ion transfer tube removal tool                 | Chamois-tipped swabs                 |
| Magnification device                           | Detergent (for example, Liquinox)    |
| Slotted screwdriver, small                     | Gloves, lint- and powder-free        |
| Sonicator                                      | Lint-free industrial tissues         |
| (Optional) Soft toothbrush (or similar tool)   | Methanol, LC/MS-grade                |
| (Optional) Tweezers, plastic (or similar tool) | MICRO-MESH polishing swab, 6000 grit |
| (Optional) Wrenches, open-end, large           | Nitrogen gas                         |
| -  | Water, LC/MS-grade                   |

#### IMPORTANT

- Prepare a clean work surface by covering the area with lint-free paper.
- Put on a new pair of lint- and powder-free gloves before starting each of these removal, cleaning, and reinstallation procedures.



**CAUTION Hot surface.** At operating temperatures above 350 °C (662 °F), the probe and API source housing can severely burn you.

- Before removing the probe or API source housing, allow the part to cool to room temperature (approximately 20 minutes) before touching it.
- If the instrument connects to an LC system, leave the solvent flow from the LC pump on while the probe cools to room temperature.

# **Removing the API Source Interface**

**\*** To remove the API source interface



**CAUTION** To avoid an electrical shock, be sure to follow the instructions in "Shutting Down the Mass Spectrometer Completely" on page 30 before continuing with this procedure.

1. Shut down and vent the system, and let it cool to room temperature.

Venting the instrument can take several minutes.

- 2. Unplug the instrument's power supply cord from the electrical outlet.
- 3. Remove the API source housing.

For instructions, refer to Chapter 2, "Setting Up the API Source," in the *LCQ Fleet Getting Started Guide*.

4. Grasp the ridges on either side of the API source interface with your fingers and carefully pull it out of the vacuum manifold (Figure 47).



Figure 47. API source interface removed from the vacuum manifold

5. Place the API source interface on the clean, lint-free work surface.

# **Cleaning the Skimmer and Tube Lens**

Chemicals accumulating on the surfaces of the skimmer and tube lens form an insulating layer that can modify the electrical fields controlling ion transmission. The skimmer and tube lens require cleaning less often than the ion sweep cone and the ion transfer tube. No tools are needed to remove or install these components.



**CAUTION** Do not scratch the outside of the skimmer cone.

To clean the skimmer and tube lens, follow these procedures:

- 1. To remove and clean the tube lens and skimmer
- 2. To reinstall the tube lens and skimmer

### • To remove and clean the tube lens and skimmer

- 1. Remove the API source interface (see page 74).
- 2. Grasp the outer ridges of the skimmer (Figure 48), pull it out of the contact ring support, and then place it on the clean, lint-free work surface.

Figure 48. Skimmer, tube lens, and API source interface cage



- 3. From the back, push the tube lens out of the contact ring support, and then place it on the work surface. If necessary, first loosen the ball plungers a little by using the small slotted screwdriver.
- 4. Clean the components as follows:

**IMPORTANT** Always use LC/MS-grade methanol and LC/MS-grade water (see Table 7 on page 49).

- a. Using a magnification device, inspect the components for any lint, particulates, and sample buildup or coatings.
- b. Soak the lint-free tissues or chamois-tipped swabs in a 50:50 solution of methanol/water, and then clean the components.
- c. Sonicate the components in methanol for 10 minutes.

**Note** If using buffers or salt solutions in the instrument, you might need to use an aqueous solution for cleaning. If using an aqueous solution, flush the items with LC/MS-grade water and then with LC/MS-grade methanol.

- d. Dry the components with nitrogen gas to make sure that all the solvent evaporates.
- 5. Using a magnification device, inspect the components for any residual lint or particulates.

**Note** Inspect the inside surfaces and edges to confirm that no lint or particulates are present. If particulates remain, use plastic tweezers or a similar tool to remove them.

### \* To reinstall the tube lens and skimmer

- 1. Reinstall the tube lens into the API source interface cage as follows:
  - a. Orient the API source interface cage as shown in Figure 49 and align the tube lens so that the lead pin points toward the correct socket in the contact ring support.
  - b. Insert the lead pin into the socket and firmly press it until it snaps into place.

Figure 49. API source interface cage





**CAUTION** Do not scratch the outside of the skimmer cone.

- 2. Reinstall the skimmer into the API source interface cage as follows:
  - a. Align the skimmer so that the lead pin points toward the socket in the contact ring support.
  - b. Insert the lead pin into the socket and firmly press it until it snaps into place.

# Cleaning the API Ion Transfer Tube, Spray Cone, and Ion Sweep Cone

Because buffer salts or high concentrations of sample can cause blockages, you must clean the bore of the ion transfer tube. If the pressure in the ion transfer tube–skimmer region (as measured by the Convectron gauge) drops considerably below 1 Torr, a blocked ion transfer tube is the likely cause.

Note You do not have to vent the system to remove the ion transfer tube.

To clean the ion transfer tube, spray cone, and ion sweep cone, follow these procedures:

- 1. To check the Convectron gauge pressure
- 2. To remove the ion transfer tube
- 3. To clean the ion transfer tube

- 4. To clean the spray cone and O-ring
- 5. To clean the ion sweep cone
- 6. To reinstall the API source interface

| For field service use only                 | Part number   |
|--|---------------|
| O-ring, Vespel <sup>™</sup> , 0.325 in. ID | 97055-20442   |
| Ion transfer tube                          | See page 112. |

#### \* To check the Convectron gauge pressure

- 1. Open the Tune Plus window (see page 28).
- 2. Choose **Setup > Vacuum** to open the Vacuum dialog box (Figure 50).

**Figure 50.** Vacuum dialog box

|  | Vacuum   | <b>—</b> ×    |
|--|--|---------------|
| Ion Trap       Close         Ion Gauge       Help         Ion Gauge Pressure (E-5 Torr): 0.73       0.73         Convectron Gauge Pressure (Torr): 0.92       0.92 | Ion Trap<br>Ion Gauge<br>Ion Gauge Pressure (E-5 Torr): 0.73<br>Convectron Gauge Pressure (Torr): 0.92 | Close<br>Help |

3. Check the reading for the Convectron Gauge Pressure. If the reading is considerably below 1 Torr, clean the ion transfer tube.

#### To remove the ion transfer tube

- 1. Turn off the flow of liquid from the LC (or other sample introduction device) to the API source as follows:
  - a. Open the Tune Plus window (see page 28).
  - b. Choose Setup > Inlet Direct Control to open the Inlet Direct Control dialog box (Figure 51).

| Inlet Direct Co | ntrol                 |            | _      | × | D                |     |
|-----------------|-----------------------|------------|--------|---|------------------|-----|
| Accela 1250     | Pump A                | ccela AS   |        | _ |                  |     |
| Pump 1          | Pump 2                |            |        |   |                  |     |
| Take            | pump unde             | er control |        |   |                  |     |
| Flow:           | 10.0                  | N/A        |        |   |                  |     |
| Time:           | N/A                   |            |        |   | Click this butto | n t |
| Inlet A:        | 100.00                | N/A        |        |   | turn off the nu  | mn  |
| Inlet B:        | 0.00                  | N/A        |        |   |                  | ΠP  |
| Inlet C:        | 0.00                  | N/A        |        |   |                  |     |
| Inlet D:        | 0.00                  | N/A        |        |   |                  |     |
| Pressure        | : N/A                 | Pressure   | Limits |   |                  |     |
| Pump<br>Release | ready<br>se injectior | ı          |        |   |                  |     |
|                 |                       |            |        | _ |                  |     |
|                 |                       | Close      | Help   |   |                  |     |

Figure 51. Inlet Direct Control dialog box for an Accela 1250 Pump



- c. Click the **Pump Off** or **Stop Pump** button.
- 2. Place the instrument's electronics service switch in the Service Mode (down) position to turn off the nonvacuum system voltages.

The service switch is located on the right side of the mass spectrometer.



**CAUTION** To avoid an electric shock, make sure that the electronics service switch is in the Service Mode (down) position before proceeding.



**CAUTION Hot surface.** The ion transfer tube operates above 250  $^{\circ}$ C (482  $^{\circ}$ F). Allow the ion sweep cone and ion transfer tube to cool to room temperature (approximately 20 minutes) before touching them.

3. After the API source cools to room temperature, remove it.

For instructions, refer to Chapter 2, "Setting Up the API Source," in the *LCQ Fleet Getting Started Guide*.

4. Grasp the outer ridges of the ion sweep cone and pull it off of the API cone seal.

Figure 52 shows the two types of ion sweep cones available on the LCQ Fleet MS. The ion sweep cone shown on the bottom has an offset orifice.



- 5. Remove the ion transfer tube as follows:
  - a. Align the flat edges (hook) of the ion transfer tube removal tool with the flat edges on the exposed tip of the ion transfer tube (Figure 53), and then turn the tool counterclockwise.

The MS Accessory Kit contains this custom tool.

b. When the tube is free of the spray cone, use the hook on the tool to pull it straight out of the API source interface.

**Figure 53.** Ion transfer tube removal tool



### ✤ To clean the ion transfer tube

**IMPORTANT** Always use LC/MS-grade methanol and LC/MS-grade water (see Table 7 on page 49).

- 1. Soak the ion transfer tube in a 50:50 solution of methanol/water for 10 minutes to remove contaminants.
- 2. Sonicate the component in water for 10 minutes.
- 3. Dry the component with nitrogen gas to make sure that all the solvent evaporates.
- 4. Reinstall the ion transfer tube into the heater block, as follows:
  - a. Using the custom removal tool, rotate the ion transfer tube clockwise as you insert it.
  - b. Continue turning the tube until it is fingertight.

### To clean the spray cone and O-ring

**IMPORTANT** Always use LC/MS-grade methanol and LC/MS-grade water (see Table 7 on page 49).

- 1. Soak the lint-free tissues or chamois-tipped swabs in a 50:50 solution of methanol/water, and then clean the exterior surface of the spray cone.
- 2. Remove and inspect the O-ring that is in the spray cone under the entrance end of the ion transfer tube (Figure 54).

Figure 54. API source interface components



- 3. Clean the O-ring with methanol or replace it if necessary (see page 78).
- 4. Using a magnification device, inspect the components for any residual lint or particulates.

**Note** Inspect the inside surfaces and edges to confirm that no lint or particulates are present. If particulates remain, use plastic tweezers or a similar tool to remove them.

5. Reinstall the O-ring in the spray cone.



**CAUTION** Be careful not to bend the ion transfer tube. Rotate the tube as you insert it.

### To clean the ion sweep cone

**IMPORTANT** Always use LC/MS-grade methanol and LC/MS-grade water (see Table 7 on page 49).

- 1. Soak the lint-free tissues or chamois-tipped swabs in a 50:50 solution of methanol/water, and then clean both sides of the ion sweep cone.
- 2. For 10 minutes, sonicate the component in either a 50:50 solution of methanol/water or a 1% solution of Liquinox in water.
- 3. Rinse the component thoroughly with water.
- 4. Sonicate the component in water for 10 minutes.
- 5. Sonicate the component in methanol for 10 minutes.
- 6. Rinse the component with methanol.
- 7. Dry the component with nitrogen gas to make sure that all the solvent evaporates.
- 8. Using a magnification device, inspect the component for any residual lint or particulates.

**Note** Inspect the inside surfaces and edges to confirm that no lint or particulates are present. If particulates remain, use plastic tweezers or a similar tool to remove them.

After you clean and reinstall the ion transfer tube, spray cone, and ion sweep cone, turn on the nonvacuum system voltages by placing the instrument's electronics service switch in the Electronics Normal (up) position. The service switch is located on the right side of the instrument.

**Tip** If you successfully unblocked the ion transfer tube, check that the Convectron gauge pressure has increased to a normal value (approximately 1 Torr). If trying this method does not clear the blockage, replace the ion transfer tube.

# **Reinstalling the API Source Interface**

### To reinstall the API source interface

- 1. Orient the API source interface as shown in Figure 47 on page 75.
- 2. Carefully insert the API source interface into the vacuum manifold until it snaps into place.
- 3. Reinstall the API source housing.

For instructions, refer to Chapter 2, "Setting Up the API Source," in the *LCQ Fleet Getting Started Guide*.

4. Start the system as described in "Starting the System after a Complete Shutdown" on page 31.

# Maintaining the Q00-L0 RF Lens

Chemicals accumulating on the surfaces of multipole Q00 segments and lens L0 form an insulating layer that can modify the electrical fields controlling ion transmission. Clean ion optic components are essential to properly operate the instrument. How frequently you clean these components depends on the type and quantity of the compounds that you analyze.

To clean or replace the Q00 rf lens components, follow these procedures:

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

Q00-L0 rf lens maintenance tasks require the following tools and supplies (see also Table 7 on page 49).

| Tools                    | Supplies                                   |
|--------------------------|--|
| 5/32 in. hex ball driver | Chamois-tipped swabs                       |
| Phillips screwdriver     | Detergent (for example, Liquinox)          |
| Magnification device     | Gloves, lint- and powder-free              |
| Slotted screwdriver      | Graduated cylinder (for use with methanol) |
| Sonicator                | Lint-free industrial tissues               |
| -                        | Methanol, LC/MS-grade                      |
| -                        | MICRO-MESH polishing swab, 6000 grit       |

| Tools | Supplies                   |
|-------|----------------------------|
| -     | Nitrogen gas               |
| -     | Water, LC/MS-grade and tap |

### **IMPORTANT**

- Prepare a clean work surface by covering the area with lint-free paper.
- Put on a new pair of lint- and powder-free gloves before starting each of these removal, cleaning, and reinstallation procedures.



**CAUTION Hot surface.** At operating temperatures above 350 °C (662 °F), the probe and API source housing can severely burn you.

- Before removing the probe or API source housing, allow the part to cool to room temperature (approximately 20 minutes) before touching it.
- If the instrument connects to an LC system, leave the solvent flow from the LC pump on while the probe cools to room temperature.

# **Removing the Q00-LO RF Lens Assembly**

| For field service use only                | Part number |
|---|-------------|
| O-ring, Viton, 3.25 in. ID, 1/8 in. thick | 00107-13000 |

### ✤ To remove the Q00-L0 rf lens assembly



**CAUTION** To avoid an electrical shock, be sure to follow the instructions in "Shutting Down the Mass Spectrometer Completely" on page 30 before continuing with this procedure.

1. Shut down and vent the system, and let it cool to room temperature.

Venting the instrument can take several minutes.

- 2. Unplug the instrument's power supply cord from the electrical outlet.
- 3. Remove the API source interface (see page 74).
- 4. Reach into the opening in the vacuum manifold (where the API source interface was) and disconnect the electrical connector to the Q00-L0 rf lens assembly.
- 5. Using the 5/32 in. hex ball driver, loosen the three hex socket-head screws that secure the API source interface to the vacuum manifold's outer cage (Figure 55).



Figure 55. Q00-L0 rf lens assembly removal

- 6. Using the 5/32 in. hex ball driver, install two of the removed hex socket-head screws into the two ejection screw holes (Figure 55) to loosen the outer cage from the vacuum manifold.
- 7. Carefully remove the Q00-L0 rf lens assembly and place it on the clean, lint-free work surface.
- 8. Remove the two hex socket-head screws from the ejection screw holes.

# Disassembling the Q00-L0 RF Lens Assembly

### ✤ To disassemble the Q00-L0 rf lens assembly

- 1. Put on a new pair of lint- and powder-free gloves.
- 2. Remove the Q00-L0 device from the back of the outer cage.

The Q00-L0 device is secured to the Q00 rf lens cage by ball plungers. Figure 56 shows the location of the ball plungers and Q00-L0 rf lens components.





# **Cleaning the Q00-LO RF Lens Assembly Components**

✤ To clean the Q00-L0 rf lens

**IMPORTANT** Always use LC/MS-grade methanol and LC/MS-grade water (see Table 7 on page 49).

- 1. Using a magnification device, inspect the components for any lint, particulates, and sample buildup or coatings.
- 2. For 10 minutes, sonicate the components in either a 50:50 solution of methanol/water or a 1% solution of Liquinox in water.
- 3. Using the 6000 grit MICRO-MESH polishing swabs, clean the bore in each lens.
- 4. Rinse the components thoroughly with water.
- 5. Sonicate the components in water for 10 minutes.
- 6. Sonicate the components in methanol for 10 minutes.

Note Put on a new pair of clean gloves before you handle the cleaned parts.

- 7. Rinse the components with methanol.
- 8. Dry the components with nitrogen gas to make sure that all the solvent evaporates.
- 9. Using a magnification device, inspect the components for any lint or particulates.

**Note** Inspect the orifices to confirm that no lint or particulates are present in the bore of the orifices. Use plastic tweezers or a similar tool to remove the lint or particulate.

# **Reassembling the Q00-L0 RF Lens Assembly**

✤ To reassemble the Q00-L0 rf lens assembly

Insert the Q00-L0 device through the back of the outer cage until it is in position.

**IMPORTANT** When reassembling the Q00-L0 rf lens assembly, remember to tighten any ball plungers that you loosened.

# **Reinstalling the Q00-L0 RF Lens Assembly**

| For field service use only             | Part number |
|--|-------------|
| O-ring, 2-148, Viton 884, 2.737 in. ID | 00107-15542 |

#### \* To reinstall the QOO-LO rf lens assembly into the vacuum manifold

- 1. Make sure that the two O-rings are properly installed on the back of the outer cage (Figure 56 on page 86).
- 2. Orient the outer cage assembly (Figure 56 on page 86).
- 3. Make sure that you removed the two hex socket-head screws from the ejection screw holes (Figure 56 on page 86).
- 4. Carefully insert the outer cage assembly into the vacuum manifold.
- 5. Using the 5/32 in. hex ball driver, tighten the three hex socket-head screws that secure the assembly to the vacuum manifold.
- 6. Reconnect the electrical connector inside the vacuum manifold (Figure 55 on page 85) as follows:
  - a. Using your fingers, align the connector's holes with the feedthrough, and then slowly push the connector into the feedthrough.
  - b. Route the connector wire below the outer cage, away from the path of the inner cage.
- 7. Reinstall the API source interface (see page 83).
- 8. Start up the system as described in "Starting the System after a Complete Shutdown" on page 31.

# Maintaining the Q0 and Q1 Ion Optics

Chemicals accumulating on the surfaces of the Q0 and Q1 ion optics form an insulating layer that can modify the electrical fields controlling ion transmission. Clean ion optic components are essential to properly operate the instrument. The cleaning frequency depends on the type and quantity of the compounds that you analyze.

To clean or replace the Q0 and Q1 ion optics components, follow these procedures:

- 1. Removing the Top Cover of the Mass Spectrometer
- 2. Removing the Vacuum Manifold's Top Cover Plate
- 3. Removing the Q0 and Q1 Ion Optics
- 4. Cleaning the Q0 and Q1 Ion Optics, Lens L1, and the Split Gate Lens
- 5. Reinstalling the Q0 and Q1 Ion Optics
- 6. Reinstalling the Top Cover of the Mass Spectrometer

Q0 and Q1 ion optics maintenance tasks require the following tools and supplies (see also Table 7 on page 49).

| Tools   | Supplies                                   |
|---|--|
| 1/4 in. hex driver                                  | Chamois-tipped swabs                       |
| 5/64 in. hex ball driver                            | Detergent (for example, Liquinox)          |
| Magnification device                                | Gloves, lint- and powder-free              |
| Phillips screwdriver                                | Graduated cylinder (for use with methanol) |
| Sonicator   | Lint-free industrial tissues               |
| (Optional) Tweezers, plastic  <br>(or similar tool) | Methanol, LC/MS-grade                      |
| -   | Nitrogen gas                               |
| -   | Water, LC/MS-grade and tap                 |

#### IMPORTANT

- Prepare a clean work surface by covering the area with lint-free paper.
- Put on a new pair of lint- and powder-free gloves before starting each of these removal, cleaning, and reinstallation procedures.



**CAUTION Hot surface.** At operating temperatures above 350 °C (662 °F), the probe and API source housing can severely burn you.

- Before removing the probe or API source housing, allow the part to cool to room temperature (approximately 20 minutes) before touching it.
- If the instrument connects to an LC system, leave the solvent flow from the LC pump on while the probe cools to room temperature.

# **Removing the Top Cover of the Mass Spectrometer**

To remove the top cover of the instrument



**CAUTION** To avoid an electrical shock, be sure to follow the instructions in "Shutting Down the Mass Spectrometer Completely" on page 30 before continuing with this procedure.

1. Shut down and vent the system, and let it cool to room temperature.

Venting the instrument can take several minutes.

- 2. Unplug the instrument's power supply cord from the electrical outlet.
- 3. Disconnect any tubing between the syringe pump or LC system and the API source.
- 4. Use the 1/4 in. hex driver to loosen the latch on the front door (Figure 57).

### Figure 57. Front door latch


5. Using the Phillips screwdriver, open the front door and loosen the two captive screws that secure the top cover (Figure 58).



6. Slide the top cover back and lift it off (Figure 59).

**Figure 59.** Top cover pushed back



# **Removing the Vacuum Manifold's Top Cover Plate**

To access the Q0 ion optics, Q1 ion optics, mass analyzer, and ion detection system, remove the top cover plate of the vacuum manifold. The top cover is held in place by gravity and by the pressure differential between vacuum and atmosphere. Five cables connect to the vacuum manifold's top cover plate.

#### \* To remove the vacuum manifold's top cover plate

- 1. Disconnect the electron multiplier HV coaxial cable at the back of the plate (Figure 60).
- 2. Use a small slotted screwdriver to loosen the screws that secure the electrometer cable, and then disconnect the cable.
- 3. Disconnect the three cables (J1, J2, and J3) connected to the top cover PCB.
- 4. Disconnect the helium tube from the top cover.

Figure 60. Electrical connections to the top cover plate of the vacuum manifold



5. Carefully lift up the top cover plate by its two handles, and place it upside down (supported on its handles) on the clean, lint-free work surface.



**CAUTION** Do not pull the cover too hard. Instead, rock it back and forth to loosen it. Lift it straight up and not at an angle to avoid damaging the bottom ion optics.

Be careful not to damage the components on the bottom side of the cover plate.

6. Cover the opening in the top of the vacuum manifold with a large, lint-free tissue.

# **Removing the QO and Q1 Ion Optics**

**\*** To remove the QO and Q1 ion optics from the top cover plate



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

- 1. Disconnect the electrical wires to multipoles Q0 and Q1, lens L1, and the split gate lens (Figure 61).
- 2. Remove the Q1 ion optics as follows:
  - a. Hold multipole Q1 and the split gate lens with one hand, and with the other hand loosen and remove the two thumbscrews that secure the Q1 support bracket to the top cover plate.

**Tip** If the thumbscrews are too tight, insert a small hex driver into the thumbscrew holes to loosen them.

- b. Slide the Q1 support bracket away from Q1 until it disengages from Q1.
- c. Remove multipole Q1 and the split gate lens and place them on the clean, lint-free work surface.
- 3. Remove the Q0 ion optics as follows:
  - a. Hold multipole Q0 and the lens L1 with one hand, and with the other hand loosen and remove the two thumbscrews that secure the Q0 support bracket to the top cover plate.

**Tip** If the thumbscrews are too tight, insert a small hex driver into the thumbscrew holes to loosen them.

- b. Slide and lift the Q0 support bracket away from multipole Q0 until it disengages from Q0.
- c. Remove Q0 and lens L1 and place them on the work surface.



Figure 61. Q0 and Q1 ion optics (exploded view) Multipole support brackets

# Cleaning the QO and Q1 Ion Optics, Lens L1, and the Split Gate Lens



**CAUTION** Do not drop or bump multipoles Q0 and Q1 against any surface.

To clean the Q0 and Q1 ion optics

**IMPORTANT** Always use LC/MS-grade methanol and LC/MS-grade water (see Table 7 on page 49).

- 1. Using a magnification device, inspect the components for any lint, particulates, and sample buildup or coatings.
- 2. Sonicate the components in a 1% solution of Liquinox in water for 10 minutes.
- 3. Soak chamois-tipped swabs in a 1% solution of Liquinox in water, and then clean the components.
- 4. Rinse the components thoroughly with water.
- 5. Sonicate the components in water for 10 minutes.
- 6. Sonicate the components in methanol for 10 minutes.
- 7. Soak chamois-tipped swabs in methanol, and then clean the components.
- 8. Rinse the components with methanol.
- 9. Dry the components with nitrogen gas to make sure that all the solvent evaporates.
- 10. Using a magnification device, inspect the components for any residual lint or particulates.

**Note** Inspect the inside surfaces and edges to confirm that no lint or particulates are present. If particulates remain, use plastic tweezers or a similar tool to remove them.

\* To clean lens L1 and the split gate lens

**IMPORTANT** Always use LC/MS-grade methanol and LC/MS-grade water (see Table 7 on page 49).

1. Using a magnification device, inspect the components for any lint, particulates, and sample buildup or coatings.

**Note** The lens surfaces in the mass spectrometer can be discolored after use, which is normal and not to be confused with sample buildup or coatings.

2. Soak the lint-free tissues or chamois-tipped swabs in a 50:50 solution of methanol/water, and then clean the components.

3. Sonicate the components in methanol for 10 minutes.

**Note** If using buffers or salt solutions in the mass spectrometer, you might need to use an aqueous solution for cleaning. If you use an aqueous solution, flush the items with LC/MS-grade water and then with LC/MS-grade methanol.

- 4. Dry the components with nitrogen gas to make sure that all the solvent evaporates.
- 5. Using a magnification device, inspect the components for any residual lint or particulates.

**Note** Inspect the inside surfaces and edges to confirm that no lint or particulates are present. If particulates remain, use plastic tweezers or a similar tool to remove them.

# **Reinstalling the QO and Q1 Ion Optics**



To reinstall the QO and Q1 ion optics

**CAUTION** Be aware of the following:

- Be careful not to bend or break the lead pins on multipoles Q0 and Q1.
- If multipole Q0 is not positioned correctly, it can be too far forward and touch the vacuum manifold.
- 1. Reinstall the Q0 ion optics as follows:
  - a. Insert lens L1 into the opening in the baffle (Figure 61 on page 94).
  - b. With one hand, hold multipole Q0 against lens L1 and press L1 against the opening in the baffle. Make sure the contact pin is up and away from the top cover plate.
  - c. With the other hand, install the Q0 support bracket at the other end of multipole Q0 by lowering and sliding it back toward Q0.
  - d. Tighten the two thumbscrews that secure the Q0 support bracket to the top cover plate.
- 2. Reinstall the Q1 ion optics as follows:
  - a. Insert the split gate lens into the opening in lens L1 (Figure 61 on page 94), and make sure that the wiring pins are horizontal.
  - b. With one hand, hold multipole Q1 against the split gate lens, and with the other hand install the Q1 support bracket at the other end of Q1 by sliding it toward Q1.
  - c. Tighten the two thumbscrews that secure the Q1 support bracket to the top cover plate.
- 3. Reconnect the electrical wires to multipoles Q0 and Q1, lens L1, and the split gate lens according to the wiring diagram (Figure 62).
- 4. Check all wires to ensure that they are secure and attached to the correct electrodes.



Figure 62. Wiring diagram for the Q0 and Q1 ion optics

# **Reinstalling the Vacuum Manifold's Top Cover**

| For field service use only  | Part number |
|---|-------------|
| Split chamber O-ring, $12.33 \times 6.65 \times 3.21$ in. $(l \times w \times h)$ | 97055-40005 |

#### \* To reinstall the vacuum manifold's top cover

- 1. Remove and discard the tissue from the vacuum manifold's top opening.
- 2. Check the vacuum manifold's split chamber O-ring for signs of wear, and replace it if necessary. Ensure that the O-ring is positioned properly.
- 3. Carefully lift the top cover plate up by its two handles and turn it over.

- 4. Orient the top cover plate so that the one or two electron multipliers, as applicable, are over the conversion dynodes.
- 5. Carefully insert the four guide posts on the bottom of the top cover plate into the holes in the vacuum manifold.
- 6. Hold the top cover plate parallel to the opening in the vacuum manifold and carefully lower it onto the opening in the vacuum manifold.



**CAUTION** Do not damage the O-ring or the components on the bottom of the top cover plate.

- 7. Reconnect the following (Figure 60 on page 92):
  - Three cables to the top cover PCB
  - One electron multiplier HV coaxial cable
  - One electrometer cable
  - Helium gas line

### **Reinstalling the Top Cover of the Mass Spectrometer**

- To reinstall the top cover of the instrument
- 1. Using the 1/4 in. hex driver on the door latch, open the front door of the instrument (Figure 58 on page 91).
- 2. Place the top cover on the instrument and slide it forward until it is flush with the front panel.
- 3. Using the Phillips screwdriver, tighten the two captive screws to secure the top cover.
- 4. Close the front door of the instrument and use the 1/4 in. hex driver to tighten the latch.
- 5. Reconnect any tubing between the syringe pump, LC pump, or LC and the API source to accommodate your instrument configuration.

# **Replacing the Electron Multiplier**

The electron multiplier has a finite lifetime; because its surface degrades over time, more voltage is required to achieve the specified gain. Several factors contribute to a decrease in the lifetime: air exposure (causes oxidation), electron flow (produces internal heat), heat, poor vacuum conditions, and water (causes arcing).

You might need to replace the electron multiplier if either of these symptoms persists:

- Excessive noise in the mass spectrum produced by the electron multiplier
- Inability of the multiplier gain calibration procedure to achieve a gain of  $4 \times 10^5$  electrons per ion with the maximum voltage supplied by the multiplier power supply

You can read the current value of the electron multiplier voltage in the Ion Detection System dialog box. In the Tune Plus window, choose **Setup > Ion Detection System**.

| For field service use only                  | Part number   |
|---|---------------|
| Electron multiplier, anode, and base shield | See page 113. |

#### To remove the electron multiplier assembly



**CAUTION** To avoid an electrical shock, be sure to follow the instructions in "Shutting Down the Mass Spectrometer Completely" on page 30 before continuing with this procedure.

1. Shut down and vent the system, and let it cool to room temperature.

Venting the instrument can take several minutes.

- 2. Unplug the instrument's power supply cord from the electrical outlet.
- 3. Remove the top cover of the instrument (see page 90).
- 4. Remove the vacuum manifold's top cover plate (see page 92).
- 5. Put on a new pair of lint- and powder-free gloves.
- 6. Using the 5/64 in. hex driver, remove the two hex socket-head screws that secure the electron multiplier to the top cover plate (Figure 63).
- 7. Detach the HV connector from the HV feedthrough to remove the electron multiplier.



Figure 63. Electron multiplier removed from the top cover plate

#### ✤ To replace the electron multiplier assembly

- 1. Insert the HV tube into the HV feedthrough (Figure 63).
- 2. Using the 5/64 in. hex driver, secure the electron multiplier to the top cover plate with the hex socket-head screws and flat washers, if provided.
- 3. Remove the tissue that is over the vacuum manifold opening.
- 4. Reinstall the top cover plate over the vacuum manifold opening (see page 98).
- 5. Reinstall the top cover of the instrument.
- 6. Start up the system as described in "Starting the System after a Complete Shutdown" on page 31.

After replacing the electron multiplier, reset and save the initial voltage setting to the appropriate value for the new multiplier, and then calibrate the electron multiplier's voltage.

#### To set the electron multiplier gain voltages

- 1. Open the Tune Plus window (see page 28).
- 2. Choose **Diagnostics > Diagnostics** to open the Diagnostics dialog box (Figure 64).
- 3. In the Tools list, select Set Device.

| Tools     Tests       Plot readback     API 1 ion       Set device     API 1 ne       Device calibration     API 2 ion       Display settings     API 2 ne       Toggles     Aux Rod       Mass calibration     Aux Rod       System evaluation     Auxiliary       Back len     Back len       Back Se     Capillary | n current (µA)<br>eedle voltage (kV)<br>nedle voltage (kV)<br>eedle voltage (V)<br>Hi Voltage (V)<br>I Low Voltage (V)<br>amplitude (V)<br>frequency (KHz)<br>gas flow (arb)<br>is (V)<br>ditipole Offset (V)<br>ction LPT Offset (V)<br>ction Offset (V)<br>heater (*C) |  | Detector settings Pulse Counting <u>Threshold:</u> 400 Set Zero the electrometer <u>Execute</u> |
|---|--|--|---|
|---|--|--|---|

Figure 64. Diagnostics dialog box showing the Set Device list

4. Scroll down the Device list and select **Multiplier Gain (V)** (Figure 65).

Figure 65. Diagnostics dialog box showing the voltage parameter for the electron multiplier

|  | Diagnostics<br>Tools Tests<br>Plot readback<br>Set device<br>RF tune<br>Device calibration<br>Display settings<br>Triggers<br>Mass calibration<br>System evaluation | Device<br>Multipoler gain (V)<br>Multipole 0 offset (V)<br>Multipole 1 offset (V)<br>Multipole RF DAC (V)<br>RF Lens offset (V)<br>Sheath gas flow (arb)<br>S-Lens RF Level (%)<br>Source heater (°C)<br>Split gate (V)<br>Sweep gas flow (arb)<br>Trap Offset (V)<br>Tube lens (V)<br>Vernier RF DAC (16-bit)<br>Value: 100.000 | E | Detector settings Pulse Counting Threshold: 6 Set Zero the electrometer Execute |
|--|---|--|---|---|
|--|---|--|---|---|

Multiplier gain

- 5. In the Value box, type -800.
- 6. Click Set.

**IMPORTANT** Follow the next procedure to save the multiplier settings or they are lost if you reset the system.

#### \* To save the electron multiplier voltage settings

1. In the Tools list, choose **Mass Calibration** to open the Mass Calibration page (Figure 66).

Figure 66. Diagnostics dialog box showing the Mass Calibration page

| Diagnostics  |  | × |
|--|--|---|
| Tools Tests  Plot readback  Set device  RF tune Device calibration Display settings Toggles Triggers System evaluation | Manual coarse calibration Calibrate current scan type Mass list: User Expected low mass: 195.10 Expected high mass: 195.10 Expected high mass: 1822.00 Deserved high mass: 1822.00 Set AGC mode Execute Estimate other calibration modes using normal scan rate calibration Execute Save |   |
|  | OK Cancel Print Help   |   |

2. Click Save, and then click OK.

To complete the process of changing the electron multiplier, calibrate the electron multiplier voltage, as described in the next procedure.

#### \* To calibrate the electron multiplier voltage

- 1. Allow the system to pump down for at least 2 hours before turning on the high voltages. (Thermo Fisher Scientific Product Support recommends 15 hours or more.)
- 2. Set up the instrument for infusing the tuning solution as described in the *LCQ Fleet Getting Started Guide*.
- Ľ
- 3. In the Tune Plus window, click the **Calibrate** icon to open the Calibrate dialog box (Figure 67).

| 💷 Calibrate                             |
|---|
| Mass Range: 💿 Normal 🔘 High             |
| Automatic Semi-Automatic Check          |
| Calibration Items                       |
| Multipole RF Frequency                  |
| Main RF Frequency                       |
| Electron Multiplier Gain                |
| Mass and Resolution for All Scan Types  |
| Isolation and Activation Waveforms      |
| Injection RF Level                      |
|   |
|   |
| Status                                  |
| A                                       |
| -                                       |
|   |
| Set Instrument to Standby when Finished |
| Start Cancel Print Help                 |

#### Figure 67. Calibrate dialog box showing the Automatic page

4. Click the **Semi-Automatic** tab (Figure 68).

Figure 68. Semi-Automatic page in the Calibrate dialog box

| Calibrate   |          |                | ×    |
|---|----------|----------------|------|
| Mas   | s Range: | Normal         | ligh |
| Automatic Semi-Automatic Check                          |          |                | -    |
| What to Calibrate                                       | Result   | Last Cal. Date |      |
| Select All  |          |                |      |
| Multipole RF Frequency                                  | -        |                | =    |
| Main RF Frequency                                       | -        |                | -    |
| Positive Ion Mode                                       |          |                |      |
| Electron Multiplier Gain                                | -        |                |      |
| Negative Ion Mode                                       |          |                |      |
| Electron Multiplier Gain                                | -        |                |      |
| Ass Calibration   |          |                |      |
| - Normal Scan Rate Types     - Enhanced Scan Pate Types | -        |                |      |
|   |          |                | -    |
| ۹ <u> </u>  |          |                | P    |
| Status  |          |                | — I  |
|   |          |                |      |
|   |          |                | ^    |
|   |          |                | -    |
|   |          |                |      |
| Set Instrument to Standby when Finished                 |          |                |      |
| Start Cancel  |          | Print          | Help |

- 5. Under both Positive Ion Mode and Negative Ion Mode, select Electron Multiplier Gain.
- 6. (Optional) Select the Set Instrument to Standby when Finished check box.
- 7. Click Start.
- 8. After the electron multiplier gain calibrations are complete, set up the instrument for operation as described in the *LCQ Fleet Getting Started Guide*.

# **Maintaining the Forepump**

Maintaining a forepump requires inspecting, adding, purging, and changing the pump oil.

Check the forepump oil often. It is a translucent light amber color. During normal operation, oil must always be visible in the oil level sight glass between the MIN and MAX marks. If the oil level is below the MIN mark, add oil. If the oil is cloudy or discolored, purge the oil to decontaminate dissolved solvents. If the pump oil is still discolored, change it. Plan to change the pump oil every 3000 hours (or about every 4 months) of operation.

Refer to the manufacturer's documentation for procedures to purge, add, and change the forepump oil.



**CAUTION** To minimize the risk of oil contamination in the vacuum system, make sure that the purging ballast is closed when venting the system to atmosphere.

| For field service use only                    | Part number |
|---|-------------|
| Forepump oil, 1 L                             | 00301-15101 |
| See the MSDS cautionary statement on page 49. |             |

# **Maintaining the Fan Filter**

Clean the fan filter every 4 months or sooner if it is dirty. The fan filter is located on the back of the instrument on the left side (when facing the back).

#### To clean the fan filter

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

# **Diagnostics**

There are two diagnostic categories—tests and tools. Use the diagnostic tests to check the functionality of the electrical subsystems and the PCBs. Use the diagnostic tools, specifically the system evaluation tools, to look at the system as a whole instrument.

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 question, you might have a hardware failure, and running the diagnostics is appropriate. If the answer is yes to one of the last two questions, the problem is probably mechanical, not electrical. Check again that alignment, configurations, and cable connections are correct before you run the diagnostics.

#### Contents

- Running General Diagnostic Tests
- Using the Diagnostic Tools

# **Running General Diagnostic Tests**

The diagnostic tests in the Tune Plus application test the major electronic circuits within the mass spectrometer and indicate whether the circuits pass or fail the tests. If there is a problem with the instrument electronics, the diagnostics can often locate it.

#### \* To run the general diagnostic tests

- 1. Open the Tune Plus window (see page 28).
- 2. Choose **Diagnostics > Diagnostics** to open the Diagnostics dialog box.
- 3. Click **Tests** at the top of the left pane to display the list of diagnostic tests (Figure 69).

| General     General     Scan device     Readbacks     API and temperatures     In Erses     Board readbacks     Source board     Analog board     Top cover board | What to Test  All tests  Shatus  RF  Characteristic constraints  RF  Shatus  RF  Shatus RF | Result           - <th>Start</th> <th></th> | Start |   |
|---|--|---|-------|---|
|   | Testing  |   |       | * |
|   |  |   |       | ~ |

Figure 69. Diagnostics dialog box showing the general test page

- 4. Select one of the following options:
  - To test all of the electronic subsystems (that is, the vacuum system, power supplies, lenses, ion detection system, and rf voltage electronics), under General, select **All**, and under What to Test, select the **All Tests** check box.
  - To test an individual subsystem, select the item corresponding to that subsystem and select the appropriate check box.
- 5. Click Start.

Testing starts and the Testing text box displays a chronological log of all diagnostic tests. After tests are completed for a specific subsystem, the Result column displays either Pass or Fail. If the diagnostics indicates a problem, contact your local Thermo Fisher Scientific field service engineer for assistance.

# **Using the Diagnostic Tools**

A subset of the diagnostic tools that are part of the Tune Plus application targets specific functions of the entire instrument. In general, these system evaluation tools do not contain pass or fail criteria nor do they rate the performance. Instead, they provide data that can be interpreted by a Thermo Fisher Scientific field service engineer. Because the system evaluations examine complex interactions, the Thermo Fisher Scientific field service engineer uses the data in conjunction with other tools and tests to form a diagnosis.

# **Running System Evaluation Tools**

#### ✤ To run the system evaluation tools

- 1. In the Tune Plus window, choose **Diagnostics** > **Diagnostics** to open the Diagnostics dialog box.
- 2. Click **Tools** to display the list of diagnostic tools (Figure 70).

Figure 70. Diagnostics dialog box showing the Tools System Evaluation page

| Diagnostics   |   | × |
|---|---|---|
| Tools     Tests       Plot readback       Set device       RF tune       Device calibration       Display settings       Toggers       Mass calibration       System evaluation | Procedure         API stability evaluation         Electron multiplier noise evaluation         Injection rf evaluation         Injection waveform evaluation         Mass drift evaluation         Multipole transmission evaluation         Resonance ejection evaluation |   |
|   |   | Ŧ |
|   | OK Cancel Print Help  |   |

3. Click **System Evaluation**, and then select the check boxes for the evaluation procedures that you want to run.

For a description of each system evaluation tool, see System Evaluation Tools.

4. Click Start.

The evaluation results appear in the Testing area.

# **System Evaluation Tools**

Table 9 lists the available system evaluation tools (procedures) for the LCQ Fleet MS in the order shown in the Tune Plus application. Several of the system evaluation tools operate when the system is in positive or negative mode, and the other tools only operate in positive mode.

**Note** If the table's last column specifies "Positive (manual)," manually set the instrument to positive mode before you run that system evaluation tool.

| System evaluation tool                  | Description   | Infusion of<br>calibration<br>solution<br>required | Positive or<br>negative<br>mode |
|---|---|--|---------------------------------|
| API Stability Evaluation                | Determines the relative standard deviation (RSD)<br>of the base peak in the current scan mode. Because<br>this procedure runs indefinitely, when you are ready<br>to end the evaluation, click <b>Stop</b> and then click<br><b>OK</b> , which closes the dialog box.                           | Yes, or any<br>analyte                             | Both                            |
| Electron Multiplier Noise<br>Evaluation | Determines the noise level in terms of the number<br>of noise pulses per scan from the multipliers,<br>dynode, and rf voltage (high mass noise). It turns<br>on and turns off the various elements to determine<br>the location of any noise if the noise level exceeds<br>the fixed threshold. | No   | Both                            |
| Injection RF Evaluation                 | Evaluates the storage efficiency of various mass ions<br>as a function of the ion trap's rf voltage during ion<br>injection, which can help identify problems with<br>the ion trap structure or rf voltage.   | Yes  | Positive<br>(manual)            |
| Injection Waveform Evaluation           | Compares the storage efficiency of the ion trap with<br>the injection waveforms turned on and off, which<br>can help identify problems with the ion trap<br>structure or injection waveform circuitry.  | Yes  | Both                            |
| Mass Drift Evaluation                   | Plots the mass of several ions and various<br>temperature sensors over time to determine the<br>amount of drift. This procedure runs indefinitely.<br>Therefore, when you are ready to end the<br>evaluation, click <b>Stop</b> and then click <b>OK</b> , which<br>closes the dialog box.      | Yes  | Positive<br>(manual)            |

Table 9. System evaluation tools and their descriptions (Sheet 1 of 2)

| System evaluation tool               | Description  | Infusion of<br>calibration<br>solution<br>required | Positive or<br>negative<br>mode |
|--------------------------------------|--|--|---------------------------------|
| Multipole Transmission<br>Evaluation | Provides information regarding sensitivity while<br>varying the multiple rf amplitude, which can help<br>determine the appropriate rf amplitude for<br>multipole transmission. | Yes  | Positive<br>(manual)            |
| Resonance Ejection Evaluation        | Determines if the resonance ejection signal is<br>functioning by turning it on and off and by<br>observing the resulting change in the spectrum.                               | Yes  | Both                            |

### Table 9. System evaluation tools and their descriptions (Sheet 2 of 2)

**6 Diagnostics** Using the Diagnostic Tools

# 7

# **Replaceable Parts**

This chapter provides the part numbers for the chemical and accessory kits that come with the LCQ Fleet MS. It also lists the replaceable and consumable parts, and their corresponding part numbers.

#### Contents

- MS Setup Kit
- Accessory Kits
- Chemical Kit
- PM Cleaning Kit (Optional)
- API Source Probes and Parts
- API Source Interface Parts
- Q00 RF Lens Parts
- Q0 and Q1 Ion Optics Parts
- Electron Multiplier
- Miscellaneous Parts

# **MS Setup Kit**

| MS Setup Kit . |  | 70111-62033 |
|----------------|--|-------------|
|----------------|--|-------------|

# **Accessory Kits**

| MS Accessory Kit      | 97055-62055 |
|-----------------------|-------------|
| Special Accessory Kit | 97055-62060 |

# **Chemical Kit**

| Chemical Kit |  | 97355-62070 |
|--------------|--|-------------|
|--------------|--|-------------|

# **PM Cleaning Kit (Optional)**

| Swabs, MICRO-MESH polishing                  | .00725-01-00027 |
|--|-----------------|
| Swabs, chamois-tipped                        | .00725-01-00028 |
| Magnifier, head-mounted opti visor           | .00725-01-00029 |
| Jeweler's loupe                              | .00725-01-00032 |
| Foam-tipped polypropylene handle, 6 in. long | .00203-99-00031 |

# **API Source Probes and Parts**

| ESI Probe Kit                               | OPTON-20011 |
|---|-------------|
| Safety Sleeve Kit                           | 70005-62015 |
| Stainless Steel Needle Kit, 32 gauge        | OPTON-53003 |
| Stainless Steel Needle Kit, 34 gauge        | OPTON-30004 |
| HESI-II Probe Kit                           | OPTON-20037 |
| High-flow Needle Insert Assembly            |             |
| (5–2000 μL/min, 32 gauge metal sample tube) | OPTON-53010 |
| Low-flow Needle Insert Assembly             |             |
| (1–10 μL/min, 34 gauge metal sample tube)   | OPTON-53011 |
| APCI Probe Kit                              | OPTON-20012 |
| APCI Probe Nozzle Assembly                  |             |

#### **ESI** Probe

| High-voltage socket O-ring                    | 00107-02550 |
|---|-------------|
| Needle seal                                   | 00950-00952 |
| Nozzle ESI nozzle O-ring, Viton, 0.676 in. ID | 00107-05710 |
| Spray needle, 26-gauge                        | 00950-00990 |

### **APCI** Probe

| Nozzle O-ring, silicone, 0.312 in. ID, 1/16 in. thick   | 00107-04500   |
|---|---------------|
| Nozzle O-ring, Viton, 0.500 in. ID, 1/16 in. thick      | 00107-05600   |
| Sample tube O-ring, Viton, 0.239 in. ID, 1/16 in. thick | 00107 - 04000 |

# **API Source Interface Parts**

| O-ring, 2-033 Viton V884, 2 in. ID, 1/16 in | 00107-01-00006 |
|---|----------------|
| O-ring, 2-039 Viton, 2.74 in. ID, 0.063 in  | 00107-12550    |
| O-ring, Vespel, graphite, 0.325 in. ID      | 97055-20442    |
| API source interface assembly               | 97055-60181    |
| Ion transfer tube                           | 97055-20517    |
| Skimmer                                     | 97055-20516    |
| Tube lens                                   | 97055-20463    |

# **Q00 RF Lens Parts**

| O-ring, 2-005, Viton, 0.101 in. ID, 0.070 in. <i>w</i>     | 00107-02456 |
|--|-------------|
| O-ring, 2-148, Viton 884, 2.737 in. ID, 0.103 in. <i>w</i> | 00107-15542 |
| Outer cage assembly  | 97055-60180 |

# **QO and Q1 Ion Optics Parts**

| Lens L1            | 97055-20022 |
|--------------------|-------------|
| Multipole bracket  | 97055-20054 |
| Multipole Q0       | 97055-60035 |
| Multipole Q1       | 97055-60154 |
| Split gate lens    | 97055-20482 |
| Thumbscrews, 10-32 | 97000-20235 |

# **Electron Multiplier**

| Electron multiplier assembly | 96000-60036 |
|------------------------------|-------------|
| Dual anode                   | 97055-20018 |

# **Miscellaneous Parts**

# **Ferrules**

Ferrule, natural PEEK, 0.027 in. ID (for use with the PEEK safety sleeve) ... 00101-18119

# **Fittings**

|          | Fitting, adapter, natural PEEK, 10-32 to 1/4-28, 0.040 in. (1.0 mm) thru-hole<br>(for the ESI probe sample inlet; Upchurch Scientific P-669) 00101-18080<br>Fitting, fingertight, natural PEEK, two wings (for the 1/16 in OD |
|----------|---|
|          | high-pressure tubing; Upchurch Scientific F-300)  |
|          | Fitting, fingertight, red, one wing (for the 1/16 in. OD high-pressure tubing;  |
|          | Upchurch Scientific F-200)  |
|          | Fitting, grounding union, stainless steel, 0.010 in. thru-hole  |
|          | (Upchurch Scientific U-435) 00101-18182   |
|          |   |
| Forepump |   |

| Forepump oil, 1 L | <br>00301-15101 |
|-------------------|-----------------|
| rorepamp on, r 2  | <br>00001 19101 |

# Sample Loops

| 5 μL, stainless steel   | 00110-22010 |
|-------------------------|-------------|
| 10 µL, stainless steel  | 00110-22012 |
| 20 µL, stainless steel  | 00110-22014 |
| 50 µL, stainless steel  | 00110-22016 |
| 100 µL, stainless steel | 00110-22018 |
| 500 µL, stainless steel | 00110-22020 |
| 1 mL, stainless steel   | 00110-22022 |

# Tubing

| Safety sleeve, natural PEEK tubing, 230 µm ID, 610 µm OD, 25.4 cm long     |             |
|--|-------------|
| (0.009 in. ID, 0.024 in. OD, 10 in. long)                                  | 00301-22806 |
| Sample tube, fused-silica, 100 μm ID, 193 μm OD                            |             |
| (0.003 in. ID, 0.008 in. OD)   | 00106-10499 |
| Tubing, red PEEK, 127 $\mu m$ ID, 1/16 in. OD (0.005 in. ID, 1.6 mm OD) $$ | 00301-22912 |
|  |             |

# Vacuum Manifold Parts

| Turbomolecular pump O-rings (Figure 17 on page 24)                | 05 |
|---|----|
|   |    |
| Viton, /./34 in. ID, 1/8 in. thick (high-vacuum inlet)            | 44 |
| Viton, 5.86 in. ID, 1/8 in. thick (interstage inlet)              | 50 |
| Viton, 4.5 in. ID, 1/8 in. thick (molecular drag inlet) 00107-145 | 00 |

# Glossary

#### A B C D E F G H I J K L M N O P Q R S T U V W X Y Z

### A

- **API ion transfer tube** A tube assembly that assists in desolvating ions that are produced by the ESI, NSI, or APCI probe.
- **API ion transfer tube offset voltage** A dc voltage applied to the ion transfer tube. The voltage is positive for positive ions and negative for negative ions.
- **API source** The sample interface between the LC and the mass spectrometer. It consists of the API probe (ESI or APCI) and API stack.
- **API stack** Consists of the components of the API source that are held under vacuum and includes the API spray shield, API ion transfer tube, API tube lens, skimmer, ion transfer tube mount, and tube lens and skimmer mount.
- **API tube lens** A lens in the API source that separates ions from neutral particles as they leave the ion transfer tube. A potential applied to the tube lens focuses the ions toward the opening of the skimmer and helps to dissociate adduct ions.
- **API tube lens offset voltage** A DC voltage applied to the tube lens. The value is normally tuned for a specific compound.

- **API tube-skimmer region** The area between the tube and the skimmer, which is surrounded by the tube lens. It is also the area of first-stage evacuation in the API source.
- **atmospheric pressure chemical ionization (APCI)** A soft ionization technique done in an ion source operating at atmospheric pressure. Electrons from a corona discharge initiate the process by ionizing the mobile phase vapor molecules. A reagent gas forms, which efficiently produces positive and negative ions of the analyte through a complex series of chemical reactions.
- **atmospheric pressure ionization (API)** Ionization performed at atmospheric pressure by using atmospheric pressure chemical ionization (APCI), electrospray ionization (ESI), or nanospray ionization (NSI).
- **atmospheric pressure photoionization (APPI)** A soft ionization technique that shows an ion generated from a molecule when it interacts with a photon from a light source.
- Automatic Gain Control<sup>™</sup> (AGC) Sets the ion injection time to maintain the optimum quantity of ions for each scan. With AGC on, the scan function consists of a prescan and an analytical scan.
- **autosampler** The device used to inject samples automatically into the inlet of a chromatograph.

# C

- **collision-induced dissociation (CID)** A method of fragmentation where molecular ions are accelerated to high-kinetic energy and then allowed to collide with neutral gas molecules such as helium or nitrogen. The collisions break the bonds and fragment the ions into smaller pieces.
- **conversion dynode** A highly polished metal surface that converts ions from the mass analyzer into secondary particles, which enter the electron multiplier.

### D

**divert/inject valve** A valve on the mass spectrometer that can be plumbed as a divert valve or as a loop injector.

# E

- **electron multiplier** A device used for current amplification through the secondary emission of electrons. Electron multipliers can have a discrete dynode or a continuous dynode.
- **electrospray (ESI)** A type of atmospheric pressure ionization that is currently the softest ionization technique available to transform ions in solution into ions in the gas phase.

electrospray ionization (ESI) See electrospray (ESI).

# Η

**heated-electrospray (H-ESI)** Converts ions in solution into ions in the gas phase by using electrospray ionization (ESI) in combination with heated auxiliary gas.

heated-electrospray ionization (H-ESI) See heatedelectrospray (H-ESI).

**high performance liquid chromatography (HPLC)** Liquid chromatography where the liquid is driven through the column at high pressure. Also known as high pressure liquid chromatography.

# I

- ion detection system A high sensitivity, on-axis system for detecting ions. It produces a high signalto-noise ratio (S/N) and allows for switching of the voltage polarity between positive ion and negative ion modes of operation. The ion detection system includes a  $\pm 15$  kV conversion dynode and a channel electron multiplier.
- **ion isolation** A step in an ion trap mass analysis where all ions but the ions of interest are ejected from the mass analyzer.
- ion isolation waveform voltage In a Thermo Scientific ion trap, a waveform voltage that is applied during the MS/SIM mode and during the precursor ion isolation step(s) of mass analysis for the MS/MS/ Full, MS<sup>n</sup>/Full, MS/MS/SRM, MS<sup>n</sup>/CRM, and all of the ZoomScan<sup>™</sup> modes (for example, all modes except MS/Full). The ion isolation waveform voltage ejects all ions but the SIM ion or precursor ion of interest.
- **ion optics** Focuses and transmits ions from the API source to the mass analyzer.
- **ion sweep cone** A removable cone-shaped metal cover that fits on top of the API ion transfer tube and acts as a physical barrier to protect the entrance of the tube.

# L

- **LC pump** A high pressure solvent pump in the liquid chromatograph (LC) that provides the pressure on the input side of a column to drive the eluent and sample through the column.
- **lens** A metal disk with a circular hole in the center that allows the ion beam to pass.

#### Μ

**mass analyzer** A device that determines the mass-tocharge ratios of ions by one of a variety of techniques.

### Ν

nanoelectrospray (nanoESI or NSI) A type of electrospray ionization (ESI) that accommodates very low flow rates of sample and solvent at 1–20 nL/min (for static nanospray) or 100–1000 nL/min (for dynamic nanospray).

nanospray ionization (nanoESI or NSI) See nanoelectrospray (nanoESI or NSI).

#### Ρ

- **precursor ion** An electrically charged molecular species that can dissociate to form fragments. The fragments can be electrically charged or neutral species. A precursor ion can be a molecular ion or an electrically charged fragment of a molecular ion. Also called a precursor ion.
- **product ion** An electrically charged product of reaction of a selected precursor ion. In general, product ions have a direct relationship to a particular precursor ion and can correlate to a unique state of the precursor ion.

### R

**rf lens** A multipole rod assembly that is operated with only radio frequency (rf) voltage on the rods. In this type of device, virtually all ions have stable trajectories and pass through the assembly.

### S

- **sample loop** A loop of calibrated volume that is used to perform flow injection analysis.
- scan Comprised of one or more microscans. Each microscan is one mass analysis (ion injection and storage/scan-out of ions) followed by ion detection. After the microscans are summed, the scan data is sent to the data system for display and/or storage. The process of ramping the amplitude of the rf and dc voltages on the multipole rods in the mass analyzer to transmit ions from the lowest mass to the highest mass of a specified scan range.

- **signal-to-noise ratio (S/N)** The ratio of the signal height (S) to the noise height (N). The signal height is the baseline corrected peak height. The noise height is the peak-to-peak height of the baseline noise.
- **skimmer** A vacuum baffle between the higher pressure tube-skimmer region and the lower pressure region. The aperture of the skimmer is offset with respect to the bore of the ion transfer tube.
- **syringe pump** A device that delivers a solution from a syringe at a specified rate.

### Т

**turbomolecular pump** A vacuum pump that provides a high vacuum for the mass spectrometer and detector system.

#### V

**vacuum manifold** A thick-walled, aluminum chamber with machined flanges on the front and sides and various electrical feedthroughs and gas inlets that encloses the API stack, ion optics, mass analyzer, and ion detection system.

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