

**Finnigan™
TSQ®
Quantum**

Hardware Manual

70111-97043 Revision A

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	Strongly Agree	Agree	Disagree	Strongly Disagree
The manual is well organized.	1	2	3	4
The manual is clearly written.	1	2	3	4
The manual contains all of the information I need.	1	2	3	4
The instructions are easy to follow.	1	2	3	4
The instructions are complete.	1	2	3	4
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Additional Comments: (Attach additional sheets if necessary.)

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Read This First

Welcome to the Thermo Electron Finnigan™ TSQ Quantum system! The TSQ Quantum is a member of the TSQ® family of Finnigan mass spectrometers.

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

This manual includes the following chapters:

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

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

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

Chapter 4: Changing API Sources contains procedures for switching ESI and APCI sources.

Chapter 5: Mass Spectrometer Maintenance outlines the maintenance procedures that you should perform on a regular basis to maintain optimum mass spectrometer performance.

Chapter 6: System Shutdown, Startup, and Reset provides procedures for shutting down and starting up the TSQ Quantum system.

Chapter 7: Diagnostics and PCB and Assembly Replacement discusses procedures for testing the major electronic circuits within the instrument and for replacing failed PCBs and assemblies.

Chapter 8: Replaceable Parts lists the replaceable parts for the mass spectrometer and data system.

Changes to the Manual and Online Help

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

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

Abbreviations

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

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

EI	electron ionization
EMBL	European Molecular Biology Laboratory
<Enter>	enter key on the terminal keyboard
ESD	electrostatic discharge
ESI	electrospray ionization
eV	electron volt
f	femto (10^{-15})
°F	degrees Fahrenheit
.fasta file	extension of a SEQUEST search database file
FOB	free on board
ft	foot
FTP	file transfer protocol
g	gram
G	giga (10^9)
GC	gas chromatograph; gas chromatography
GC/MS	gas chromatograph / mass spectrometer
GND	electrical ground
GPIB	general-purpose interface bus
GUI	graphical user interface
h	hour
<i>h</i>	height
HPLC	high-performance liquid chromatograph
HV	high voltage
Hz	hertz (cycles per second)
ICIS™	Interactive Chemical Information System
ICL™	Instrument Control Language™
ID	inside diameter
IEC	International Electrotechnical Commission
IEEE	Institute of Electrical and Electronics Engineers
in.	inch
I/O	input/output
k	kilo (10^3 , 1000)
K	kilo (2^{10} , 1024)
KEGG	Kyoto Encyclopedia of Genes and Genomes
kg	kilogram

<i>l</i>	length
L	liter
LAN	local area network
lb	pound
LC	liquid chromatograph; liquid chromatography
LC/MS	liquid chromatograph / mass spectrometer
LED	light-emitting diode
μ	micro (10 ⁻⁶)
m	meter
mm	milli (10 ⁻³)
M	mega (10 ⁶)
M+	molecular ion
MB	Megabyte (1 048 576 bytes)
MH+	protonated molecular ion
min	minute
mL	milliliter
mm	millimeter
MS	mass spectrometer; mass spectrometry
MS	MS ⁿ power: where n = 1
MS/MS	MS ⁿ power: where n = 2
MS ⁿ	MS ⁿ power: where n = 1 through 10
<i>m/z</i>	mass-to-charge ratio
n	nano (10 ⁻⁹)
NCBI	National Center for Biotechnology Information (USA)
NIST	National Institute of Standards and Technology (USA)
OD	outside diameter
Ω	ohm
p	pico (10 ⁻¹²)
Pa	pascal
PCB	printed circuit board
PID	proportional / integral / differential
P/N	part number
P/P	peak-to-peak voltage

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

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

MSⁿ (in this manual) MSⁿ (in the online Help)

10⁵ (in this manual) 10⁵ (in the online Help)

Typographical Conventions

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

- Data input
- Boxed information
- Topic headings

Data Input

Throughout this manual, the following conventions indicate data input and output via the computer:

- Messages displayed on the screen are represented by capitalizing the initial letter of each word and by italicizing each word.
- Input that you enter by keyboard is represented in **bold face letters**. (Titles of topics, chapters, and manuals also appear in bold face letters.)
- For brevity, expressions such as “choose **File > Directories**” are used rather than “pull down the File menu and choose Directories.”
- Any command enclosed in angle brackets < > represents a single keystroke. For example, “press <F1>” means press the key labeled *F1*.
- Any command that requires pressing two or more keys simultaneously is shown with a plus sign connecting the keys. For example, “press <Shift> + <F1>” means press and hold the <Shift> key and then press the <F1> key.
- Any button that you click on the screen is represented in bold face letters and a different font. For example, “click on **Close**”.

Boxed Information

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

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

Boxed information can be of the following types:

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

Topic Headings

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

Chapter 1

Chapter Name

1.2 Second Level Topics

Third Level Topics

Fourth Level Topics

Fifth Level Topics

Safety Precautions

Observe the following safety precautions when you operate or perform service on the mass spectrometer.

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

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

Shut Down the Mass Spectrometer and Disconnect It From Line Power Before You Service It.

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

Respect Heated Zones.

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

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

The presence of atmospheric oxygen in the API source when the mass spectrometer is On could be unsafe. (TSQ Quantum system automatically turns off the mass spectrometer when you open the API source; however, it is best to take this added precaution.)

Make Sure You Have Sufficient Nitrogen For Your API Source.

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

Provide an Adequate Fume Exhaust System and Contain Waste Streams.

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

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

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

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

Use Care When Changing Vacuum Pump Oil.

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

Solvent and Gas Purity Requirements

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

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

Solvent Source	Telephone Number
Mallinckrodt/Baker, Inc.	Tel: (800) 582-2537 Fax: (908) 859-6905
Burdick & Jackson, Inc.	Tel: (800) 368-0050 Fax: (231) 725-6216
EMD Chemicals, Inc.	Tel: (800) 222-0342 Fax: (856) 423-4389

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

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

Service Philosophy

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

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

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

Reply Cards

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

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

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

Chapter 1

Introduction

The TSQ Quantum is a member of the TSQ[®] family of Finnigan[™] mass spectrometers. The TSQ Quantum is an advanced analytical instrument that includes a syringe pump, a divert/inject valve, a mass spectrometer, and the Xcalibur[®] data system. See Figure 1-1. In a typical analysis, a sample can be introduced in any of the following ways:

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

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



Figure 1-1. Finnigan TSQ Quantum system

The TSQ Quantum mass spectrometer consists of an atmospheric pressure ionization (API) source, ion guides, triple-stage mass analyzer, and ion detection system. The ion guides, 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 process used to ionize the sample is referred to as the *ionization mode*. The ions produced in the API source are transmitted by the ion guides into the mass analyzer, where they are separated according to their mass-to-charge ratio. The polarity of the potentials applied to the lenses in the API source and ion guides determines whether positively charged ions or negatively charged ions are transmitted to the mass analyzer. You can configure the TSQ Quantum mass spectrometer to analyze positively or negatively charged ions (called the positive or negative *ion polarity mode*).

The ions produced in the API source are filtered according to their mass-to-charge ratios (mass analyzed) by the triple-stage mass analyzer, which can perform either one or two stages of mass analysis. When the TSQ Quantum system is operated as a conventional mass spectrometer with one stage of mass analysis, the sample is ionized in the ion source and the ion products are subjected to mass analysis in the first rod assembly. The resulting mass-selected ions are then transmitted (through the second and third rod assemblies) to the ion detection system.¹

When the TSQ Quantum system is operated as a tandem mass spectrometer, as before, the sample is ionized in the ion source and is mass analyzed by the first rod assembly. In this case, however, mass-selected ions exiting the first rod assembly are allowed to collide with an inert gas in the second rod assembly and fragment to produce a new set of ion products. (The second rod assembly is surrounded by a chamber called the *collision cell*. The collision cell can be pressurized with an inert gas.) The secondary ion products then undergo a further mass analysis in the third rod assembly and selected ions are detected. In this mode, two stages of analysis are performed. In the first stage, ion production occurs in the ion source, and the first mass analyzer carries out mass analysis. In the second stage of analysis, formation of new ionic species occurs in the collision cell, and the second mass analyzer performs mass analysis. Two stages of mass analysis yield far greater chemical specificity than a single stage can achieve, because two discrete but directly related sets of masses can be selected and determined.

TSQ Quantum systems can be used to elucidate the structures of pure organic compounds and the structures of the components within mixtures. Each ionic fragment of a molecule formed in the ion source and separated in a first stage of mass analysis can be further fragmented and then further separated in a second stage of mass analysis to build up an entire structure for the molecule, piece by piece. Thus, all pathways for the formation and fragmentation of each ion in the mass spectrum can be investigated.

¹ The instrument can also be used as a single-stage mass spectrometer by transmitting the ions through the first and second rod assemblies followed by mass analysis in the third rod assembly.

The two stages of mass analysis, with resultant reduction of chemical noise in the final mass spectrum, make analysis very selective and sensitive.

Each sequence of single or triple-stage mass analysis of the ions is called a *scan*. The TSQ Quantum system uses several different *scan modes* and different *scan types* to filter, fragment, or transmit ions in the mass analyzer. The ability to vary the scan mode and scan type, as well as the ionization and ion polarity modes, affords the user great flexibility in the instrumentation for solving complex analytical problems.

This chapter contains the following sections:

- Ion Polarity Modes
- Ionization Modes
- Scan Modes
- Scan Types
- Data Types

1.1 Ion Polarity Modes

You can operate the TSQ Quantum system in either of two *ion polarity modes*: positive or negative. Both positively charged and negatively charged ions are formed in the API source of the mass spectrometer. The TSQ Quantum system can control whether positive ions or negative ions are transmitted to the mass analyzer for mass analysis by changing the polarity of the potentials applied to the API source and ion guides. The ion guides are located between the API source and the mass analyzer.

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

1.2 Ionization Modes

You can operate the TSQ Quantum system in either of two ionization modes:

- Electrospray Ionization (ESI)
- Atmospheric Pressure Chemical Ionization (APCI)

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

Electrospray Ionization

The *electrospray ionization (ESI) mode* transforms ions in solution into ions in the gas phase.¹ Many samples that previously were not suitable for mass analysis (for example, heat-labile compounds or high molecular weight compounds) can be analyzed by the use of ESI. ESI can be used to analyze any polar compound that makes a preformed ion in solution. The term *preformed ion* can include adduct ions. For example, polyethylene glycols can be analyzed from a solution containing ammonium acetate because of adduct formation between the NH_4^+ ions in the solution and oxygen atoms in the polymer. With ESI, the range of molecular weights that can be analyzed by the TSQ Quantum system is greater than 100,000 u, due to multiple charging. ESI is especially useful for the mass analysis of polar compounds, which include: biological polymers (for example, proteins, peptides, glycoproteins, and nucleotides); pharmaceuticals and their metabolites; and industrial polymers (for example, polyethylene glycols).

In ESI, ions are produced and analyzed as follows:

1. The sample solution enters the ESI needle, to which a high voltage is applied.
2. The ESI needle sprays the sample solution into a fine mist of droplets that are electrically charged at their surface.
3. The electrical charge density at the surface of the droplets increases as solvent evaporates from the droplets.
4. The electrical charge density at the surface of the droplets increases to a critical point known as the Rayleigh stability limit. At this critical point, the droplets divide into smaller droplets because the electrostatic

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

repulsion is greater than the surface tension. The process is repeated many times to form very small droplets.

5. From the very small, highly charged droplets, sample ions are ejected into the gas phase by electrostatic repulsion.
6. The sample ions enter the mass spectrometer and are analyzed.

Figure 1-2 shows the steps in the formation of ions from highly charged droplets.

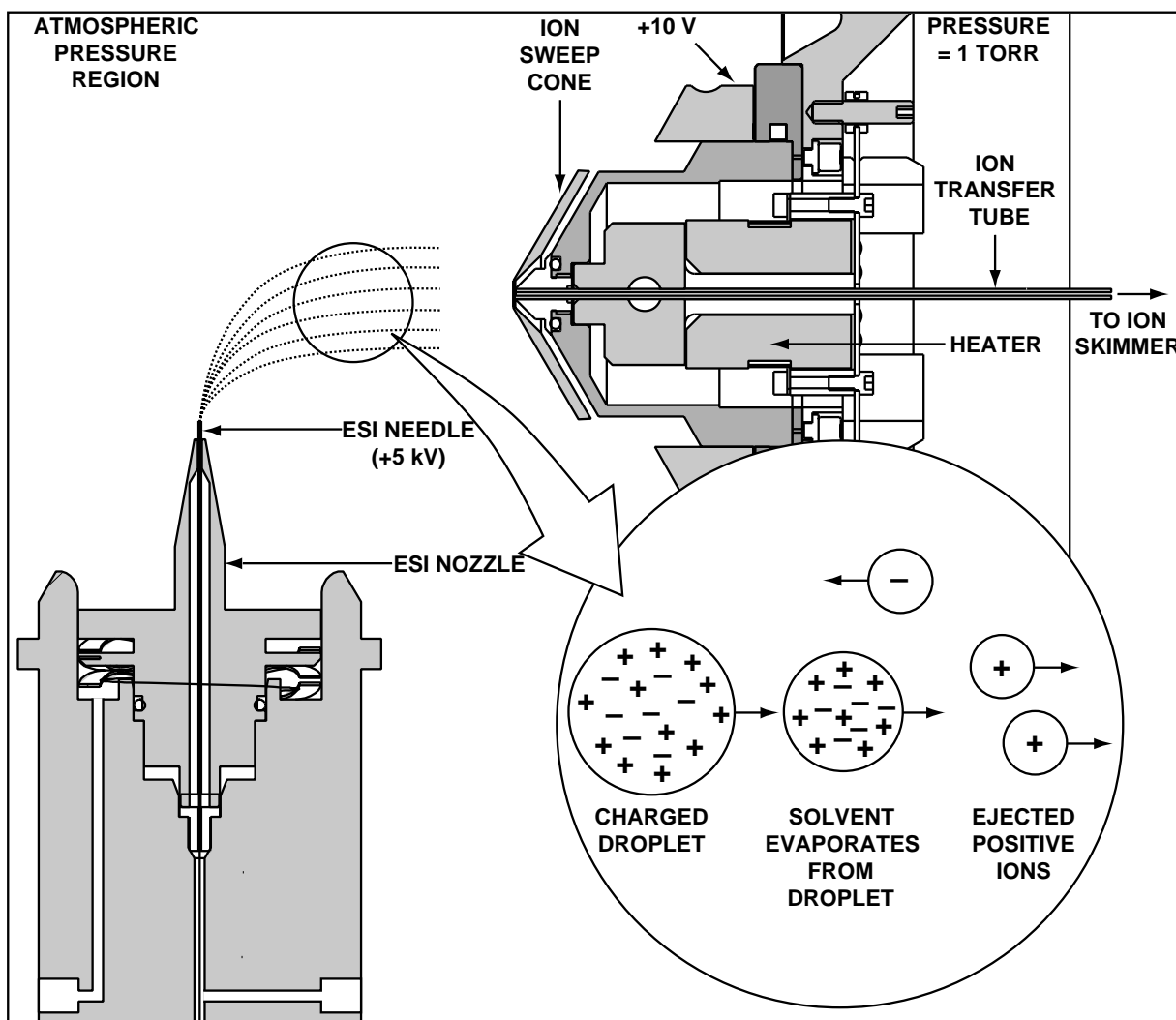


Figure 1-2. ESI process in the positive ion polarity mode

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

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

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

Organic solvents such as methanol, acetonitrile, and isopropyl alcohol are superior to water for ESI. Volatile acids and bases are good, but salts above 10 mM concentration and strong acids and bases are extremely detrimental.

The rules for achieving a good electrospray are:

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

Atmospheric Pressure Chemical Ionization

Atmospheric pressure chemical ionization (APCI) is a soft ionization technique, but not as soft as ESI. APCI is used to analyze compounds of medium polarity that have some volatility.

In APCI, ions are produced and analyzed as follows:

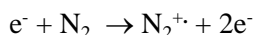
1. The APCI nozzle sprays the sample solution into a fine mist of droplets.
2. The droplets are vaporized in a high temperature tube (the vaporizer).
3. A high voltage is applied to a needle located near the exit end of the tube. The high voltage creates a corona discharge that forms reagent ions through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

Figure 1-3 shows the APCI process for a positive adduct ion formation.

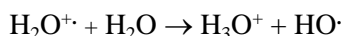
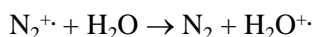
APCI is a gas phase ionization technique. Therefore, the gas phase acidities and basicities of the analyte and solvent vapor play an important role in the APCI process.

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

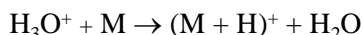
Primary ion formation



Secondary ion formation



Proton transfer



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

APCI is typically used to analyze small molecules with molecular weights up to about 1500 u. APCI is a very robust ionization technique. It is not affected by minor changes in most variables, such as changes in buffers or changes in buffer strength.

You can use APCI in positive or negative ion polarity mode. For most molecules, the positive-ion mode produces a stronger ion current. This is especially true for molecules with one or more basic nitrogen (or other basic)

atoms. An exception to the general rule is that molecules with acidic sites, such as carboxylic acids and acid alcohols, produce more negative ions than positive ions.

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

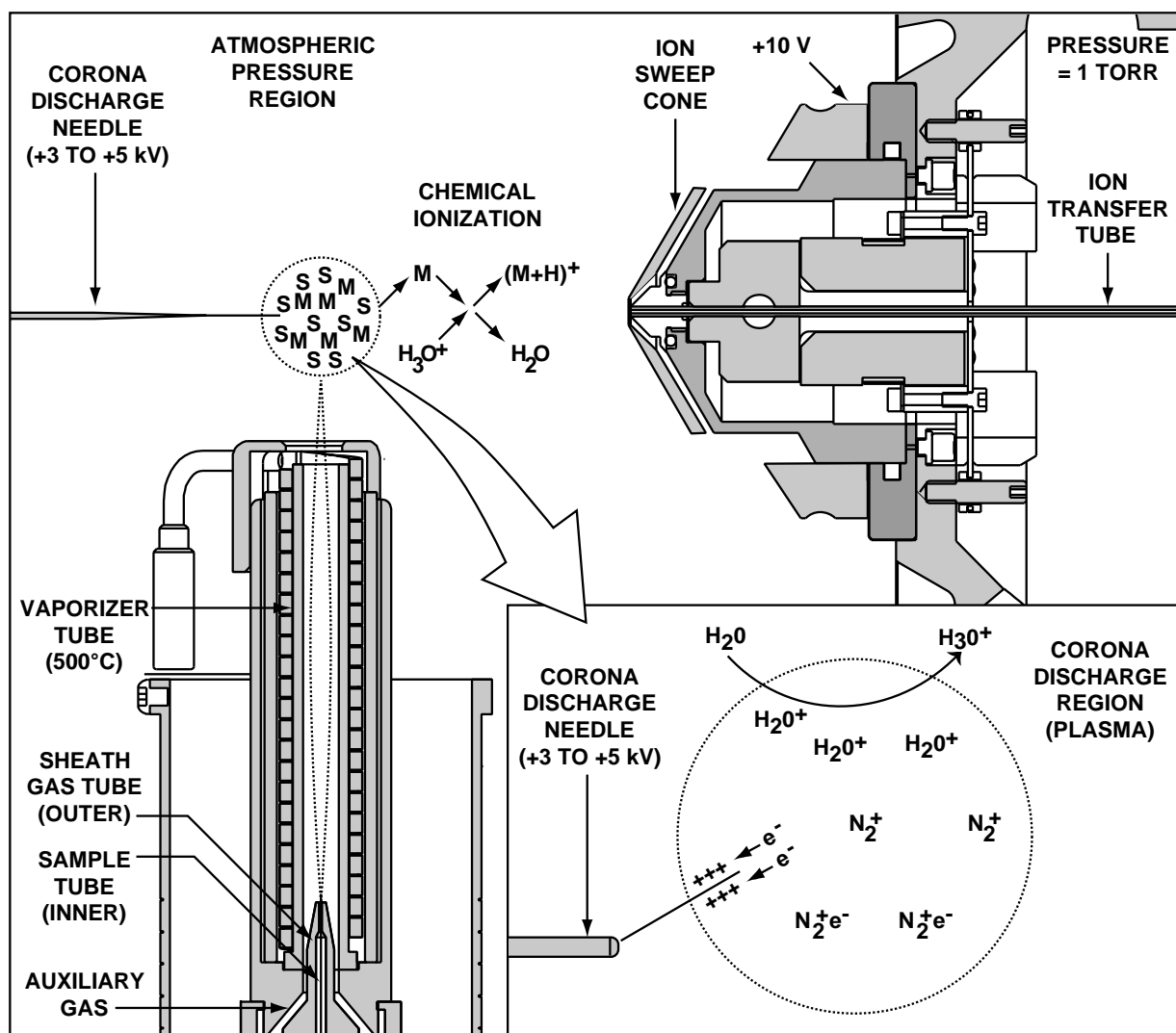


Figure 1-3. APCI process in the positive ion polarity mode

1.3 Scan Modes

The TSQ Quantum system can be operated in a variety of scan modes. The most commonly used scan modes can be divided into two categories: single mass spectrometry (MS) scan modes and MS/MS scan modes. The scan modes in each category are as follows:

- MS scan modes: Q1MS and Q3MS Scan Modes
- MS/MS scan modes: Product Scan Mode, Parent Scan Mode, Neutral Loss Scan Mode
- Data Dependent Scan Mode

The scan modes that can be employed depend on the number and type of rod assemblies and the voltages applied to the rod assemblies.

The TSQ Quantum mass analyzer has three rod assemblies.¹ The first and third rod assemblies, Q1 and Q3, are *HyperQuads*[™] (hyperbolic-profile quadrupoles), and the second rod assembly, Q2, is a square-profile quadrupole.

Rod assemblies can be operated in either of two capacities:

- Ion transmission devices
- Mass analyzers

If only RF voltage is applied, a rod assembly serves as an ***ion transmission device*** that passes all ions within a large range of mass-to-charge ratios (virtually all ions present).

When both RF and dc voltages are applied to a rod assembly, the separation of ions of different mass-to-charge ratios occurs. This separation allows the rod assembly to serve as a ***mass analyzer***.

On the TSQ Quantum instrument, the hyperquad rod assemblies can be operated with RF and dc voltages or with only RF voltage. That is, Q1 and Q3 can act either as mass analyzers or ion transmission devices. The Q2 rod assembly always operates with only RF voltage. Thus, Q2 is always an ion transmission device. For a summary of how the rod assemblies function in several of the major scan modes, refer to Table 1-1.

¹ A rod assembly is a regular array of metal rods. Refer to the topic **Mass Analyzer** on page 2-24 for a discussion of the rod assemblies used on the TSQ Quantum instrument.

Table 1-1. Functions of the rod assemblies in different scan modes

Scan Mode	Q1 Hyperquad	Q2 Collision Cell	Q3 Hyperquad
Q1MS	Scan ^a	Pass all ions ^b	Pass all ions
Q3MS	Pass all ions	Pass all ions	Scan
Product	Set ^d	Fragment ions ^c , then pass all fragments	Scan
Parent	Scan	Fragment ions, then pass all fragments	Set
Neutral Loss	Scan	Fragment ions, then pass all fragments	Scan

^aScan = full scan or transmission of selected ions

^bPass all ions or fragments = pass ions or fragments within a wide range of mass-to-charge ratios

^cFragment ions = collisions with argon gas cause ions to fragment

^dSet = set to pass ions of a single mass-to-charge ratio or a set of mass-to-charge ratios

Q1MS and Q3MS Scan Modes

In the *Q1MS and Q3MS scan modes*, only one stage of mass analysis is performed. The mass spectrum obtained is equivalent to that from an instrument with a single mass analyzer. In the one stage of analysis, ions formed in the ion source enter the analyzer assembly. One of the mass analyzers (Q1 or Q3) is scanned to obtain a complete mass spectrum. The other rod assemblies (Q2 and Q3, or Q1 and Q2, respectively) act as ion transmission devices. In the Q1MS scan mode, Q1 is used as the mass analyzer; in the Q3MS scan mode, Q3 is used as the mass analyzer.

Product Scan Mode

In the *Product scan mode*, two stages of analysis are performed. In the first stage, ions formed in the ion source enter Q1, which is set to transmit ions of one mass-to-charge ratio. Ions selected by this first stage of mass analysis are called *parent ions*. (Thus, Q1 is referred to as the *Parent mass analyzer*, and the mass-to-charge ratio of ions transmitted by the Parent mass analyzer is referred to as the *Parent set mass*.) Parent ions selected by Q1 then enter Q2, which is surrounded by the collision cell.

Note. When the first, second, and third rod assemblies are being discussed as pieces of hardware, it is convenient to refer to them as Q1, Q2, and Q3, respectively. However, when their function in MS/MS scan modes is being discussed, it often adds clarity to refer to them as the Parent mass analyzer, collision cell (ion transmission device surrounded by the collision cell), and Product mass analyzer, respectively.

In the second stage of analysis, ions in the collision cell can fragment further to produce **product ions**. Product ions can be produced by unimolecular decomposition of metastable ions or by interaction with argon collision gas present in the collision cell. This latter step is known as **collision-induced dissociation (CID)**. Ions formed in the collision cell enter Q3 (the **Product mass analyzer**) for the second stage of mass analysis. Q3 is scanned to obtain a mass spectrum that shows the product ions produced from the fragmentation of the selected parent ion.

A mass spectrum obtained in the Product scan mode (**Product mass spectrum**) is the mass spectrum of a selected parent ion.

The Product scan mode is illustrated in Figure 1-4.

Experiments in which the Product scan mode is employed (**Product experiments**) can be used to survey complex organic mixtures (such as biological samples), to sequence peptides, to perform metabolic screening, or to perform quantitative analysis of specific target compounds.

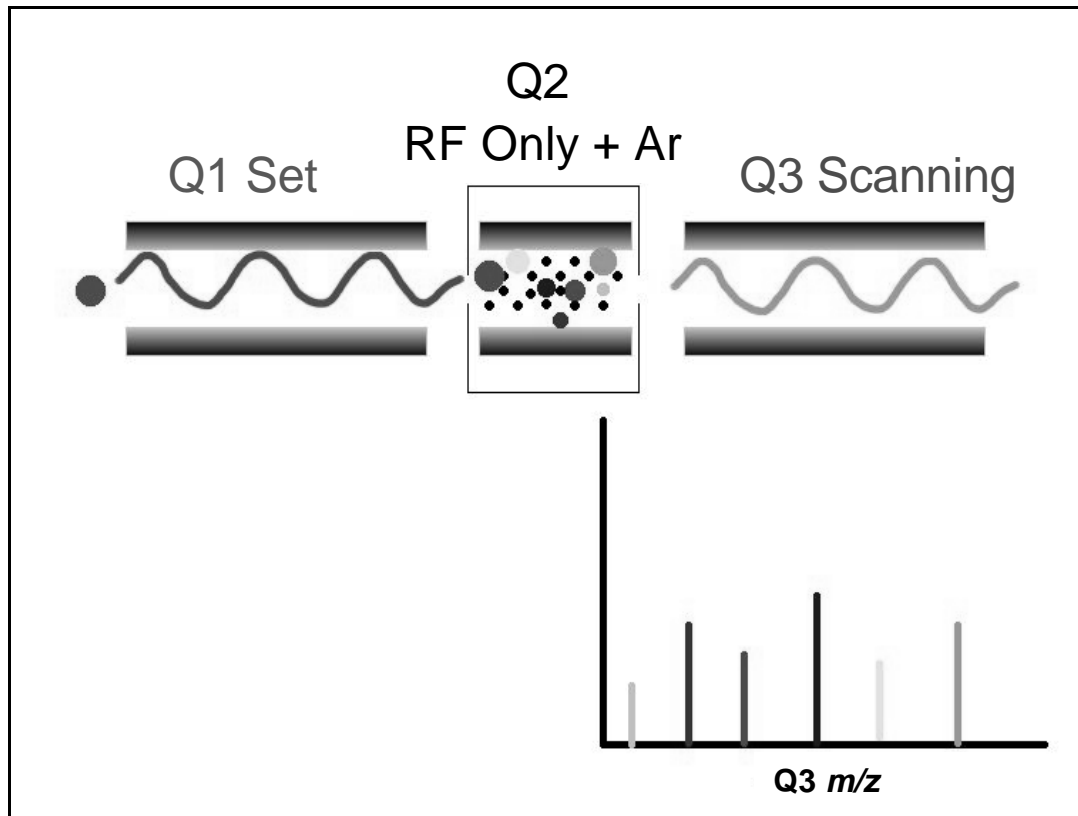


Figure 1-4. Illustration of Product scan mode

Parent Scan Mode

The *Parent scan mode* also uses two stages of analysis. In the first stage, ions formed in the ion source are introduced into the Parent mass analyzer, which is scanned to transmit parent ions sequentially into the collision cell.

In the second stage of analysis, in the collision cell, parent ions can fragment to produce product ions by unimolecular decomposition of metastable ions or by collision-induced dissociation. Ions formed in the collision cell enter the Product mass analyzer, which transmits a selected product ion. (The mass-to-charge ratio of ions transmitted by the Product mass analyzer is referred to as the *Product set mass*.)

The resultant spectrum shows all the parent ions that fragment to produce the selected product ion. Note that for a mass spectrum obtained in the Parent scan mode (*Parent mass spectrum*), data for the mass-to-charge ratio axis are obtained from Q1 (the parent ions), whereas data for the ion intensity axis are obtained from Q3 (the product ion being monitored).

Parent scan mode is illustrated in Figure 1-5.

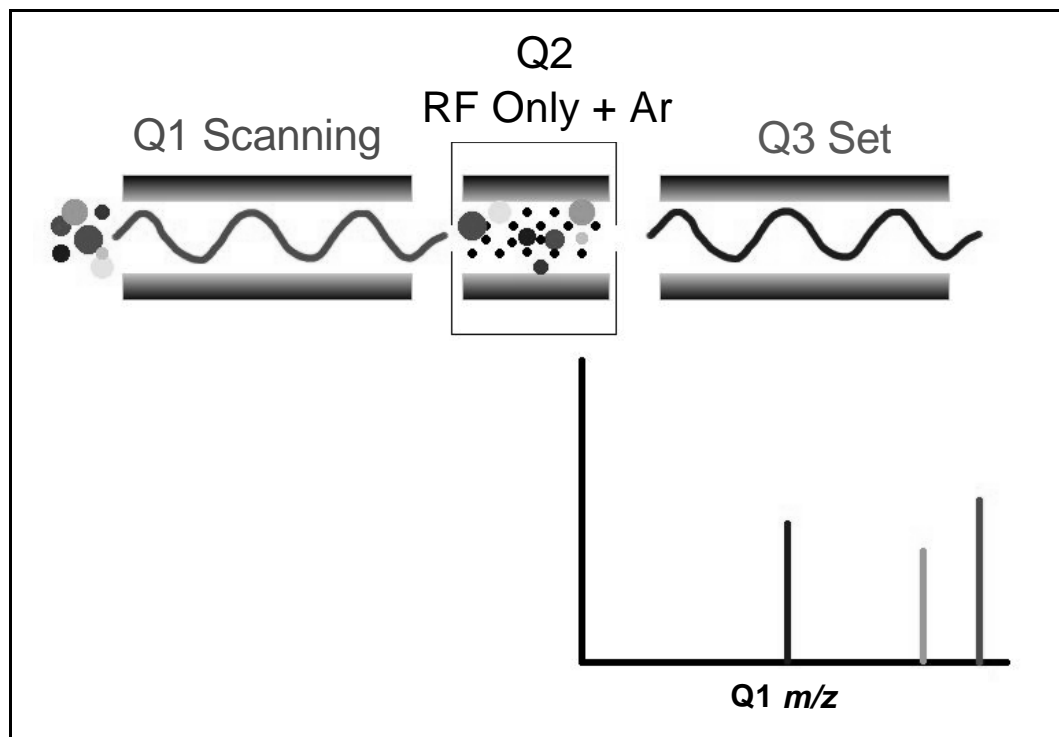


Figure 1-5. Illustration of the Parent scan mode

Experiments in which the Parent scan mode is employed (*Parent experiments*) can be used in structure and fragmentation studies as well as in survey analyses of mixtures. In general, Parent experiments detect all compounds that decompose to a common fragment. Therefore, the experiments are useful for the rapid detection of a series of structural homologs (for example, substituted aromatics, phthalates, steroids, or fatty acids) that have a common fragment ion (for example, m/z 149 for the phthalates).

Neutral Loss Scan Mode

In the *Neutral Loss scan mode*, the two mass analyzers (Q1 and Q3) are linked together so that they are scanned at the same rate over mass ranges of the same width. The respective mass ranges, however, are offset by a selected mass, such that the Product mass analyzer scans a selected number of mass units **lower** than the Parent mass analyzer.

Thus, in the Neutral Loss scan mode, there are two stages of mass analysis. In the first stage, ions formed in the ion source are separated by mass-to-charge ratio by the Parent mass analyzer and are introduced sequentially into the collision cell.

In the second stage of analysis, ions admitted to the collision cell can fragment further to produce product ions by metastable ion decomposition or by CID. These product ions are then separated by mass-to-charge ratio by the Product mass analyzer. Neutral loss scan mode is illustrated in Figure 1-6. Examples of compounds with a common neutral loss fragment are shown in Figure 1-7.

For an ion to be detected, between the time the ion leaves Q1 and enters Q3, it must lose a neutral moiety whose mass (the *Neutral Loss mass*) is equal to the difference in the mass ranges being scanned by the two mass analyzers. Thus, a spectrum is obtained (a *Neutral Loss mass spectrum*) that shows all the parent ions that lose a neutral species of a selected mass.

Note that a Neutral Gain (or Association) experiment can also be performed in which the mass range scanned by Q3 is offset by a selected mass **above** that scanned by Q1.

For a Neutral Loss (or Neutral Gain) mass spectrum, as for a Parent mass spectrum, data for the mass-to-charge ratio axis are obtained from Q1 (the parent ion), whereas data for the ion intensity axis are obtained from Q3 (the product ion being monitored).

Experiments in which the Neutral Loss scan mode is used (*Neutral Loss experiments*) are useful when a large number of compounds is being surveyed for common functionality. Neutral moieties are frequently lost from substituent functional groups (for example, CO₂ from carboxylic acids, CO from aldehydes, HX from halides, and H₂O from alcohols).

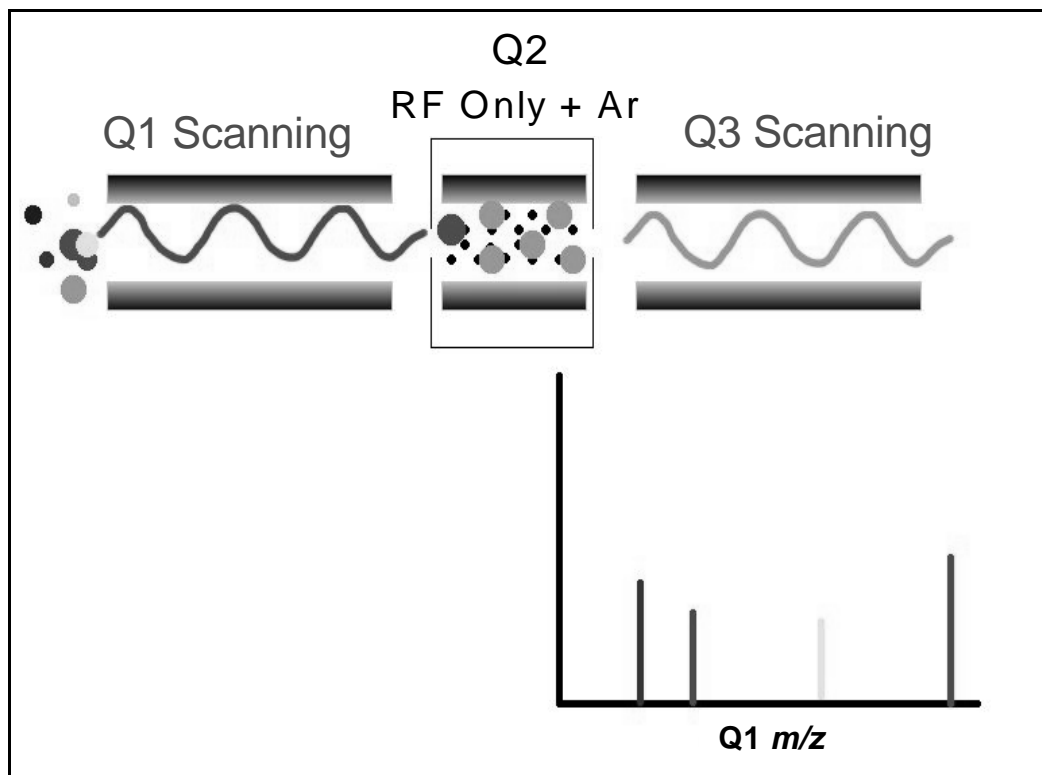


Figure 1-6. Illustration of the Neutral Loss scan mode

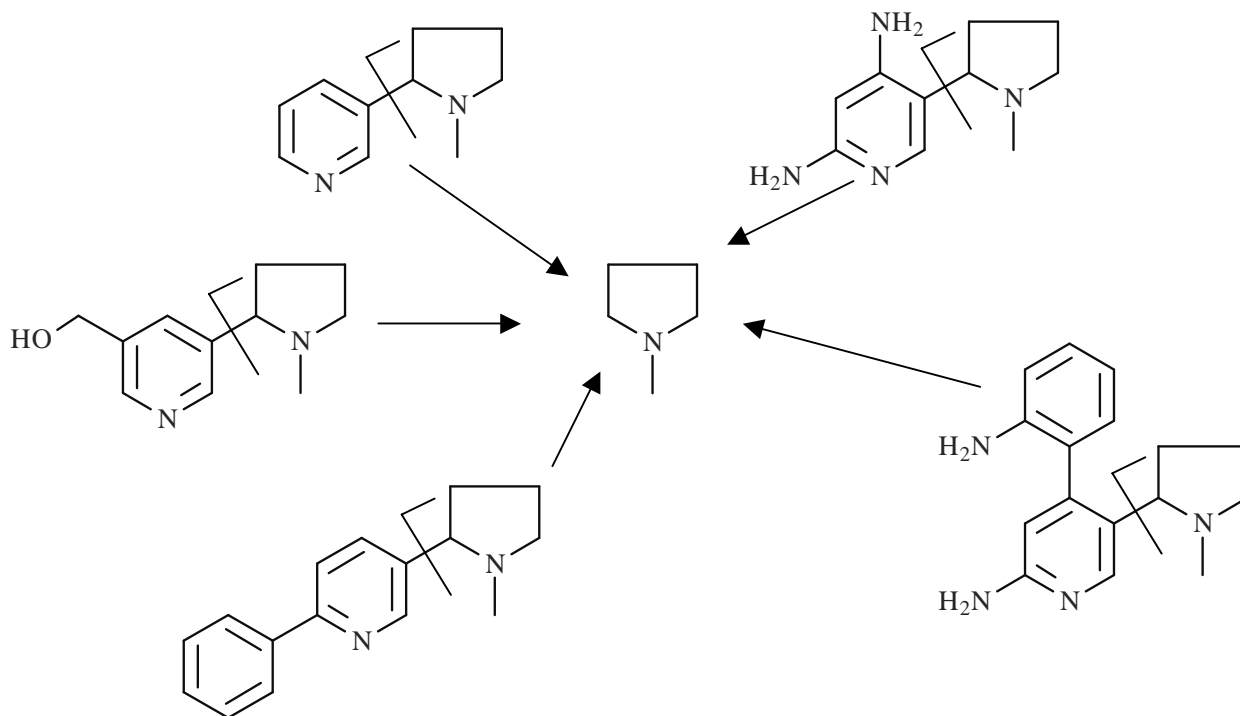


Figure 1-7. Examples of compounds with a common neutral-loss fragment

Data Dependent Scan Mode

The TSQ Quantum system uses the information in a *Data Dependent scan mode* experiment to make decisions about the next step of the experiment automatically—without input from a user. In Data Dependent scan mode you specified criteria to select one or more ions of interest to perform subsequent scans on, such as MS/MS. You can approach the setup of Data-Dependent experiments in either of two ways:

- If you have some idea of what the parent ion is, or if you expect a certain kind of parent, you can set up a list of possible parent ions. Then, when one of the parent ions you specified is detected, you can acquire product spectra and analyze the information. Conversely, you can also set up a list of ions that you do *not* want to be selected for fragmentation.
- If you have little information about your compound, you can set up the parameters of a Data Dependent experiment so that if the intensity of the ion signal is above a specified threshold, the TSQ Quantum system generates product spectra. Later, you can decide if the information is useful.

Because a data dependent scan needs to use a target ion from a previous scan, the first scan event cannot be a data dependent scan.

1.4 Scan Types

TSQ Quantum systems can be operated with a variety of scan types. The most common scan types are as follows:

- Full Scan
- Selected Ion Monitoring (SIM)
- Selected Reaction Monitoring (SRM)

Full Scan

The *full scan scan type* provides a full mass spectrum of each analyte. With full scan, the scanning mass analyzer is scanned from the first mass to the last mass, without interruption, in a given scan time.

Full scan experiments are used to determine or confirm the identity of unknown compounds or the identity of each component in a mixture of unknown compounds. (Generally, a full mass spectrum is needed to determine the identity of an unknown compound.) For example, you would use a full scan to determine the molecular weight of each component of a tryptic digest of a protein, because you would not know what masses to expect in the digest mixture.

The full scan scan type gives you more information about an analyte than does SIM, but a full scan does not yield the sensitivity that can be achieved by the other two scan types. With full scan, you spend less time monitoring the signal for each ion than you do in SIM or SRM. Thus, full scan provides greater information but lower sensitivity than the other two scan types.

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

Selected Ion Monitoring

Selected ion monitoring (SIM) is a technique in which a particular ion or set of ions is monitored. SIM experiments are useful in detecting small quantities of a target compound in a complex mixture when the mass spectrum of the target compound is known. Thus, SIM is useful in trace analysis and in the rapid screening of a large number of samples for a target compound.

Because only a few ions are monitored, SIM can provide lower detection limits and greater speed than the full scan modes. Lower detection limits are achieved because more time is spent monitoring significant ions that are

known to occur in the mass spectrum of the target analyte. Greater speed is achieved because only a few ions of interest are monitored; regions of the spectrum that are empty or have no ions of interest are not monitored.

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

Selected Reaction Monitoring

In *selected reaction monitoring (SRM)*, a particular reaction or set of reactions, such as the fragmentation of an ion or the loss of a neutral moiety, is monitored.

In SRM, a limited number of parent / product-ion pairs are monitored. In Product-type experiments, a parent ion is selected as usual, but generally only one product ion is monitored. SRM experiments are normally conducted with the Product scan mode.

Like SIM, SRM allows for the very rapid analysis of trace components in complex mixtures. However, because two sets of ions are being selected, the specificity obtained in SRM can be much greater than that obtained in SIM. Any interfering compound would not only have to form an ion source product (parent ion) of the same mass-to-charge ratio as the selected parent ion from the target compound, but that parent ion would also have to fragment to form a product ion of the same mass-to-charge ratio as the selected product ion from the target compound.

1.5 Data Types

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

- Profile Data Type
- Centroid Data Type

Profile Data Type

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

Centroid Data Type

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

Chapter 2

Functional Description

This chapter describes the principal components of the TSQ Quantum instrument and their respective functions. The principal components are as follows:

- Autosampler (optional)
- Liquid Chromatograph (optional)
- Syringe Pump
- Divert/Inject Valve
- Mass Spectrometer
- Data System

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

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

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

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

Upon entering the mass spectrometer, sample molecules are ionized by electrospray ionization (ESI) or atmospheric pressure chemical ionization (APCI). The ion guides focus and accelerate the resulting sample ions into the mass analyzer where they are analyzed according to their mass-to-charge ratios. The sample ions are then detected by an ion detection system that produces a signal proportional to the number of ions detected. The ion current signal from the ion detection system is received and amplified by the system electronics and is then passed on to the data system for further processing, storage, and display. The data system provides the primary TSQ Quantum user interface.

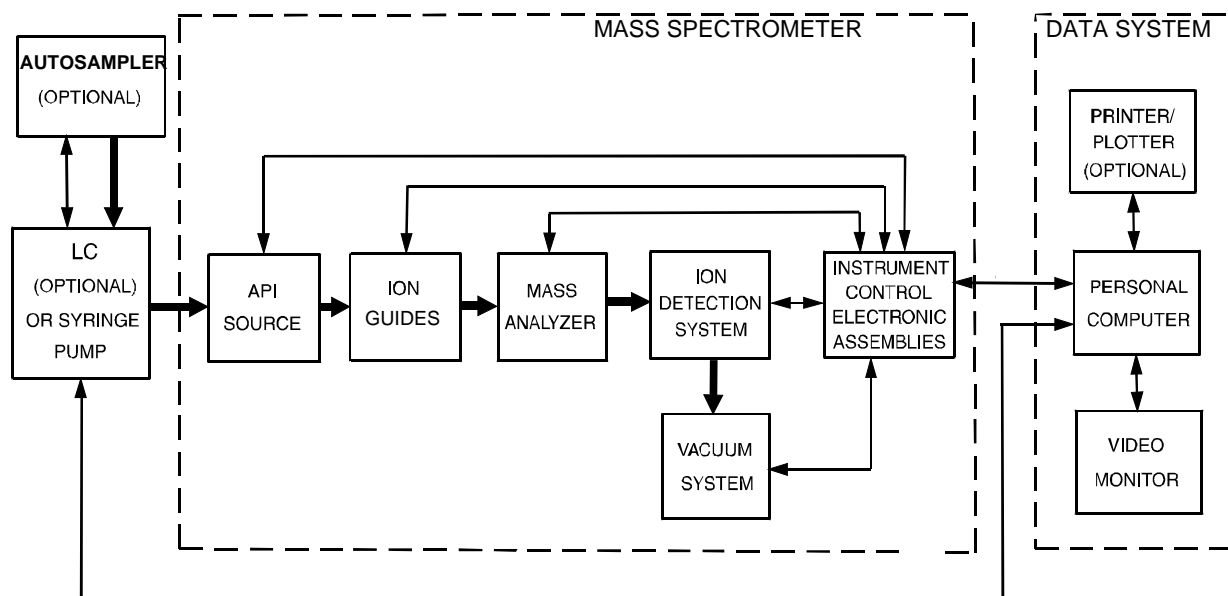


Figure 2-1. Functional block diagram of the TSQ Quantum system. The broad, single-headed arrows represent the flow of sample molecules through the instrument. The narrow, double-headed arrows represent electrical connections.

2.1 Autosampler

The (optional) *autosampler* is used to inject samples automatically into the LC inlet. The Thermo Electron Finnigan¹ SPECTRASYSTEM[®] AS3000 and AS3500; the Thermo Electron Finnigan Surveyor[®]; the Waters 2690, 2695, and 2795; and the Agilent^{®2} 1100 autosamplers can be controlled directly from the TSQ Quantum data system computer. With an autosampler, you can automate your LC/MS analyses.

Autosampler Start/Stop signals with the TSQ Quantum system are provided by contact closure. Refer to the **Finnigan TSQ Quantum Getting Connected** manual for information on connecting an autosampler to the TSQ Quantum system by contact closure.

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

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

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

¹ Formerly Thermo Separation Products (TSP)

² Formerly Hewlett-Packard (HP)

2.2 Liquid Chromatograph

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

Thermo Electron Finnigan SPECTRASYSYSTEM P2000 and P4000; the Thermo Electron Finnigan Surveyor; the Waters 2690, 2695, and 2795; and the Agilent 1100 LCs and the corresponding UV detectors can be controlled directly from the TSQ Quantum data system computer. Refer to the **Finnigan TSQ Quantum Getting Connected** manual for information on connecting an LC to the TSQ Quantum system.

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

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

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

2.3 Syringe Pump

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

You can start and stop the syringe pump from the Syringe Pump dialog box, which can be reached from the Tune Master window (which is available by choosing **Start > Programs > Xcalibur > Quantum Tune**). Refer to the Tune Master online Help for instructions on operating the syringe pump from the data system.

You can also start and stop the syringe pump by pressing the syringe pump button. You can run the syringe pump in Purge mode, in which the flow rate is 5% of the syringe volume per minute, by holding down the button.

The **syringe pump LED** (see Figure 2-5) is illuminated green whenever the syringe pump is pumping. The LED is illuminated yellow if the syringe pump is at the end of its travel.

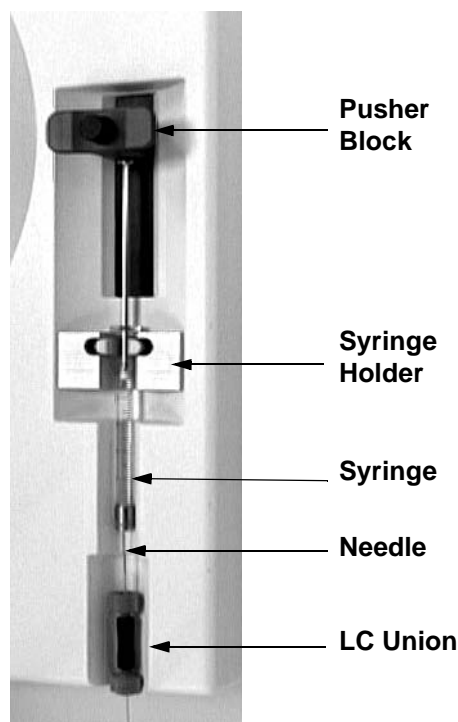


Figure 2-2. Syringe pump

2.4 Divert/Inject Valve

The Rheodyne® 7750E-185 *divert/inject valve* is a motorized, stainless steel, six-port valve that switches between two positions: Load and Inject. The divert/inject valve is located on the front of the TSQ Quantum instrument above the API source. See Figure 2-3. You can configure (plumb) the divert/inject valve as a loop injector (for flow injection analysis) or as a divert valve. See Figure 2-4. Procedures for plumbing the valve in the loop injector or divert valve configuration are given in the **Finnigan TSQ Quantum Getting Started** manual.

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

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

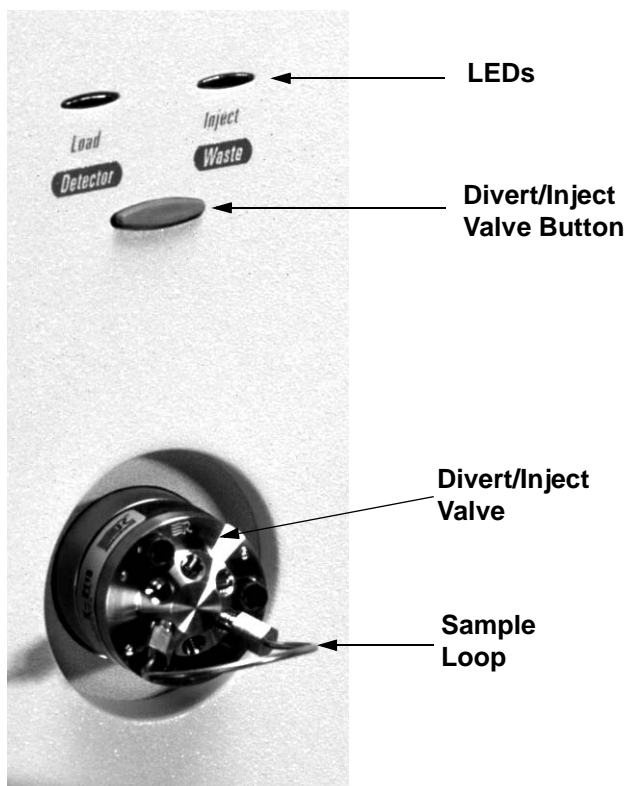
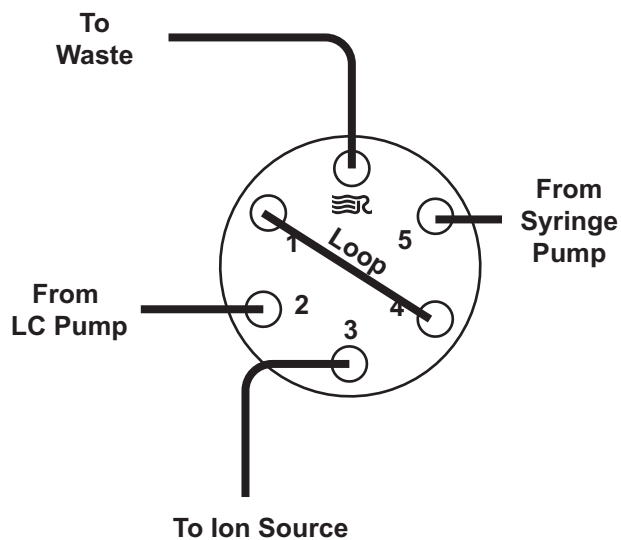


Figure 2-3. Divert/inject valve

Plumbed as a Loop Injector



Plumbed as a Divert Valve

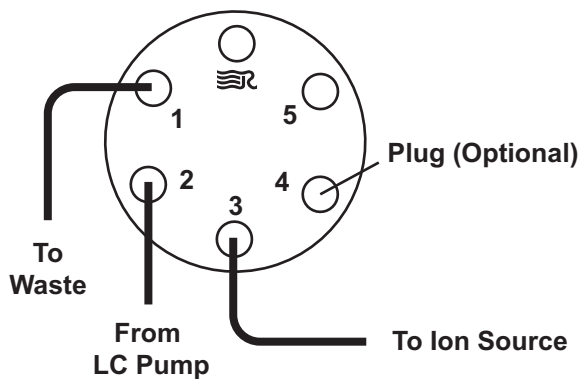


Figure 2-4. Divert/inject valve plumbed as a loop injector and as a divert valve

2.5 Mass Spectrometer

The *mass spectrometer* provides sample ionization and mass analysis of injected samples or samples eluted from a liquid chromatograph. The TSQ Quantum mass spectrometer uses a triple-quadrupole mass analyzer with an ion source external to the mass analyzer. Several important features of the TSQ Quantum mass spectrometer are as follows:

- High sensitivity and resolution
- m/z 30 to 1500 mass range
- ESI and APCI ionization modes
- Positive and negative ion polarity modes
- MS and MS/MS scan modes
- Full scan, SIM, SRM, and data dependent scan types

The *mass spectrometer* includes the following components:

- Controls and Indicators
- API Source
- Ion Guides
- Mass Analyzer
- Ion Detection System
- Vacuum System and Inlet Gasses Hardware
- Cooling Fans
- Electronic Assemblies

Controls and Indicators

Six light-emitting diodes (LEDs) are located at the upper right side of the front panel of the mass spectrometer. See Figure 2-5.

The **Power LED** is illuminated green whenever power is supplied to the vacuum system and electronic assemblies of the mass spectrometer.

The **Vacuum LED** is illuminated yellow when the turbomolecular pump is nearly at speed (80% of its operating speed of 750 MHz) and it is safe to turn on the ion gauge. The Vacuum LED is illuminated green whenever the pressure in the analyzer chamber, as measured by the ion gauge, is at or below the value required to enable high voltages to the mass analyzer (8×10^{-6} Torr). The Vacuum LED is off if the turbomolecular pump is not at speed.

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

The **System LED** is illuminated yellow whenever the mass spectrometer is in Standby (that is, high voltage is not supplied to the API source, mass analyzer, or ion detection system, but the mass spectrometer power is on). The System LED is also illuminated yellow if the safety interlock switch is open, or if the APCI vaporizer heater cable or the ESI interlock plug is not connected. The System LED is illuminated green whenever the high voltage is enabled and the system is in the On state. High voltage is enabled if the analyzer chamber is below 8×10^{-6} Torr, the safety interlock switch is closed, and the APCI vaporizer heater cable or ESI interlock plug is connected.

The **Scan LED** flashes blue whenever the mass spectrometer is On and is scanning ions.

The **Syringe Pump LED** is illuminated green whenever the syringe pump is pumping. The Syringe Pump LED is illuminated yellow when the pump reaches the end of its travel. The LED is extinguished when the syringe pump is not on and is not at the end of its travel.

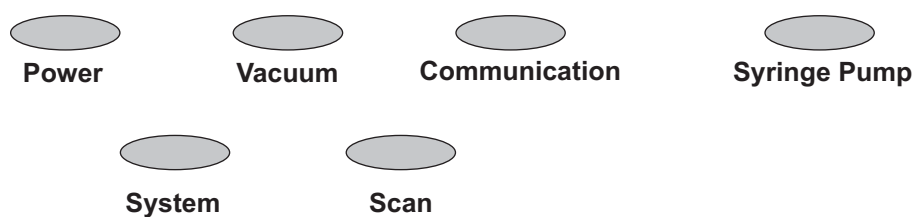


Figure 2-5. Front panel LEDs of the mass spectrometer

Two additional LEDs and a push-button switch are located on the front panel above the divert/inject valve. See Figure 2-6. When the divert/inject valve is set up for loop injections, the divert/inject valve button toggles the valve between load and inject modes and the labels *Load* and *Inject* apply.

When the divert/inject valve is set up for divert valve operation, the divert/inject valve button toggles the LC flow between the mass spectrometer and the waste container and the labels *Detector* and *Waste* apply.

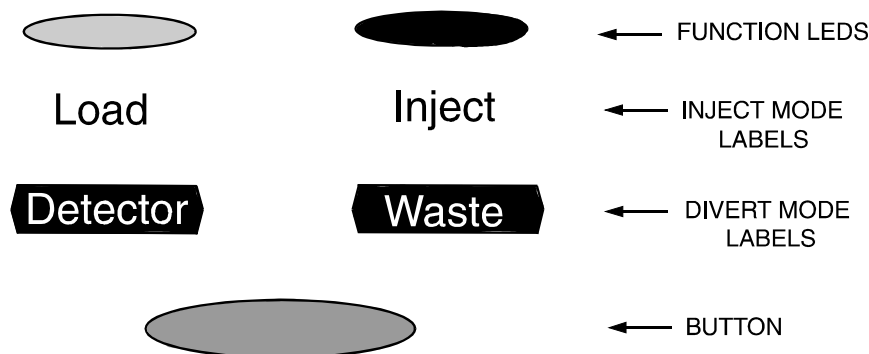


Figure 2-6. Divert/inject valve button and LEDs

The **main power circuit breaker switch** (labeled *Main Power*) is located on the power panel at the lower right corner of the right side panel of the mass spectrometer. See Figure 2-7. In the Off (O) position, the circuit breaker removes all power to the mass spectrometer, including the vacuum pumps. In the On (I) position, power is supplied to the mass spectrometer. In the standard operational mode, the circuit breaker is kept in the On (I) position.

The **electronics service switch** (labeled *Service*) is located next to the main power circuit breaker on the power panel (Figure 2-7). In the Service Mode position the switch removes power to all components of the mass spectrometer other than the vacuum system. In the Operating Mode position power is supplied to all non-vacuum system components of the mass spectrometer.

The **vacuum service switch** (labeled *Vacuum*) is located next to the electronics Service switch on the power panel (Figure 2-7). In the Service Mode position the switch removes power to the forepump, turbomolecular pump, 24 V power supply, cooling fans, Vent Delay PCB, and vent valve. The vent valve then opens after a delay time. In the Operating position power is supplied to the forepump, turbomolecular pump, 24 V power supply, cooling fans, and Vent Delay PCB. The vent valve is then closed.

Note. To shut off all power to the mass spectrometer in an emergency, place the main power circuit breaker switch (labeled *Main Power*) in the Off (O) position.

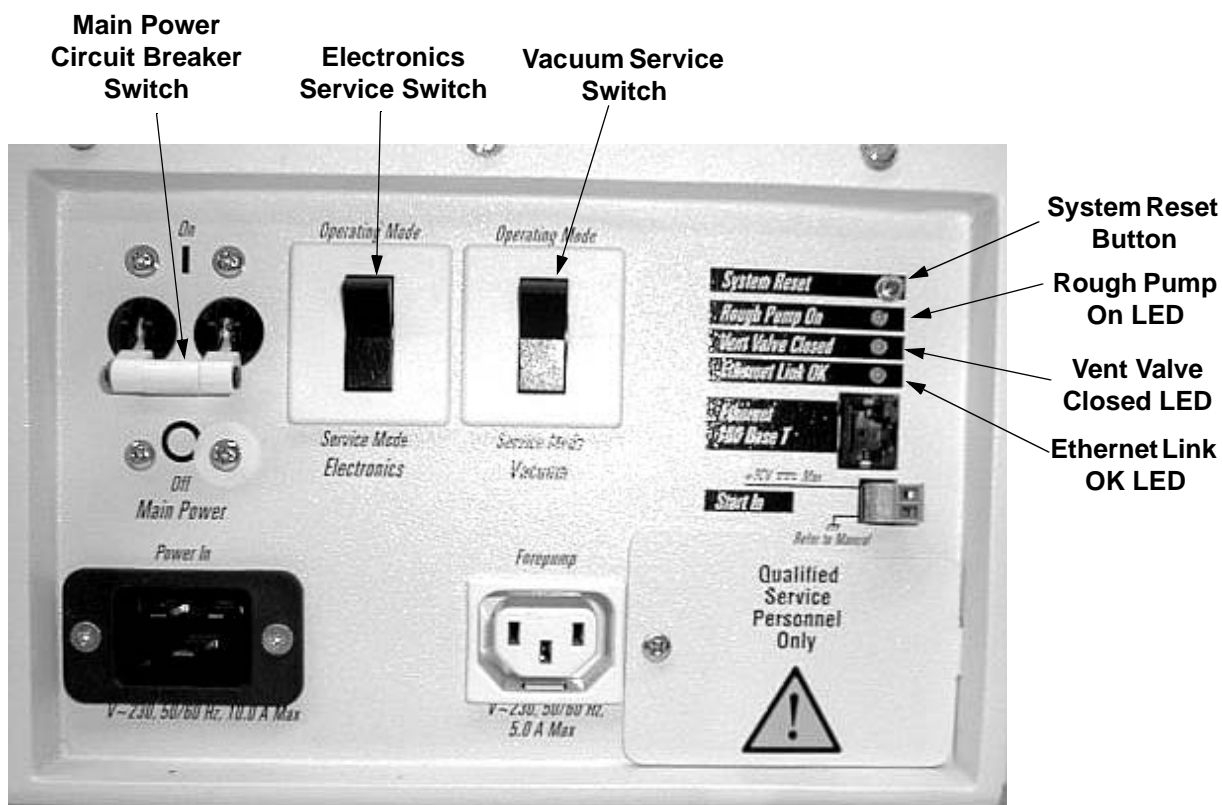


Figure 2-7. Power panel, showing switches and LEDs

The **System Reset button** is also located on the power panel. Pressing the System Reset button takes the 5 V logic to ground and causes the embedded computer on the System Control PCB to reboot. The TSQ Quantum software is then reloaded from the data system. Refer to the topic **Resetting the Mass Spectrometer** on page 6-10 for information on resetting the mass spectrometer.

Four LEDs are located on the power panel: The **Rough Pump On LED** is illuminated green when the rough pump current sensor detects current to the forepump. The LED is off when the rough-pump current sensor does not detect current to the forepump. If the current sensor detects a loss of current when the TSQ Quantum is on, the vacuum system will vent.

The **Vent Valve Closed LED** is illuminated green whenever the vent valve current sensor detects current through the vent valve and the vent valve is closed. The LED is off when the vent valve is open.

The **Ethernet Link OK LED** is illuminated green when the System Control PCB is communicating with the data system PC. The LED is off when there is no communication between the System Control PCB and the data system PC.

API Source

The *atmospheric pressure ionization (API) source* forms gas phase sample ions from sample molecules that are contained in solution. The API source also serves as the sample interface between the LC and the mass spectrometer. You can operate the API source in either the electrospray ionization (ESI) or atmospheric pressure chemical ionization (APCI) mode.

The API source consists of the following:

- API Source Housing
- API Probe (ESI Probe or APCI Probe)
- Ion Source Interface

API Source Housing

The *API source housing* seals the atmospheric pressure region of the API source. See Figure 2-8 and Figure 2-9. The ESI and APCI probes mount inside the housing (There are separate housings for ESI and APCI). The API source housing includes a lid to access the API probe, two nitrogen gas inlets for the sheath gas and auxiliary gas, an inlet for the sample line, a drain port for waste liquid, and high voltage electrical connections for the electrospray needle (ESI) or for the vaporizer and corona discharge needle (APCI). A high voltage *safety interlock switch* turns off the following voltages when the API source housing lid is open:

- ESI spray voltage (or APCI corona discharge voltage)
- All API source and lens voltages, including the ion transfer tube offset voltage
- RF and DC voltages on Q00 and Q0 ion guides, Q1 and Q3 hyperquads, and Q2 collision cell

The above voltages are also turned off if the APCI vaporizer cable (APCI mode) or the ESI interlock plug (ESI mode) is not plugged into the APCI vaporizer high voltage connector on the TSQ Quantum instrument.



Figure 2-8. ESI source housing and ESI probe



Figure 2-9. APCI source housing and APCI probe

API Probe

The **API probe** is the source of sample ionization. You need to switch probes when you change ionization modes. Two API probes are available with the TSQ Quantum system:

- ESI Probe
- APCI Probe

ESI Probe

The **ESI probe** produces charged aerosol droplets that contain sample ions. See Figure 2-10. The ESI probe accommodates liquid flows of 1 $\mu\text{L}/\text{min}$ to 1 mL/min without splitting.

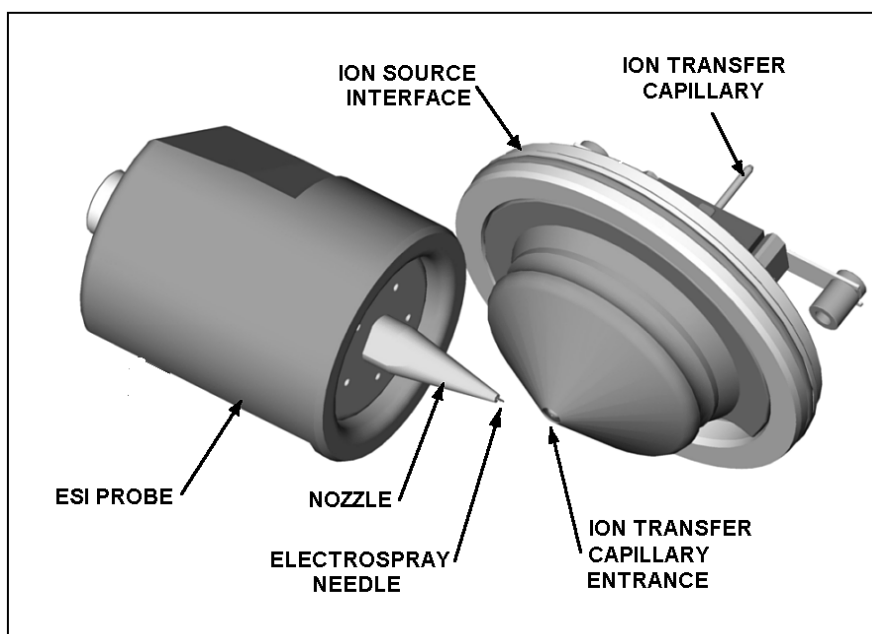


Figure 2-10. ESI probe and ion source interface

The ESI probe includes the ESI sample tube, needle, nozzle, and manifold. See Figure 2-11. Sample and solvent enter the ESI probe through the sample tube. The **sample tube** is a short section of 0.1 mm ID fused-silica tubing that extends from a fitting secured to the ESI source housing, through the ESI probe and into the ESI needle, to within 1 mm from the end of the ESI needle. The ESI **needle**, to which a large negative or positive voltage is applied (typically ± 3 to ± 5 kV), sprays the sample solution into a fine mist of charged droplets. The ESI **nozzle** directs the flow of sheath gas and auxiliary gas at the droplets. The ESI **manifold** houses the ESI nozzle and needle and includes the sheath gas and auxiliary gas plumbing. The **sheath gas plumbing** and **auxiliary gas plumbing** deliver dry nitrogen gas to the nozzle.

The ESI probe has inlets for the introduction of sample solution, sheath gas, and auxiliary gas into the API source. The **sheath gas** is the inner coaxial nitrogen gas that sprays (nebulizes) the sample solution into a fine mist as it exits the sample tube. Typical sheath gas flow rates for ESI are 10 to 30 units for sample flow rates of less than 10 $\mu\text{L}/\text{min}$, and 30 to 60 units for sample flow rates greater than 400 $\mu\text{L}/\text{min}$. When you tune the TSQ Quantum system, you should adjust the sheath gas flow rate until the ion signal is stable.

The **auxiliary gas** is the outer coaxial nitrogen gas that assists the sheath gas in the nebulization and evaporation of sample solutions. The auxiliary gas also helps lower the humidity in the ion source. Typical auxiliary gas flow rates for ESI and APCI are 10 to 20 units. Auxiliary gas is usually not needed for sample flow rates below 50 $\mu\text{L}/\text{min}$.

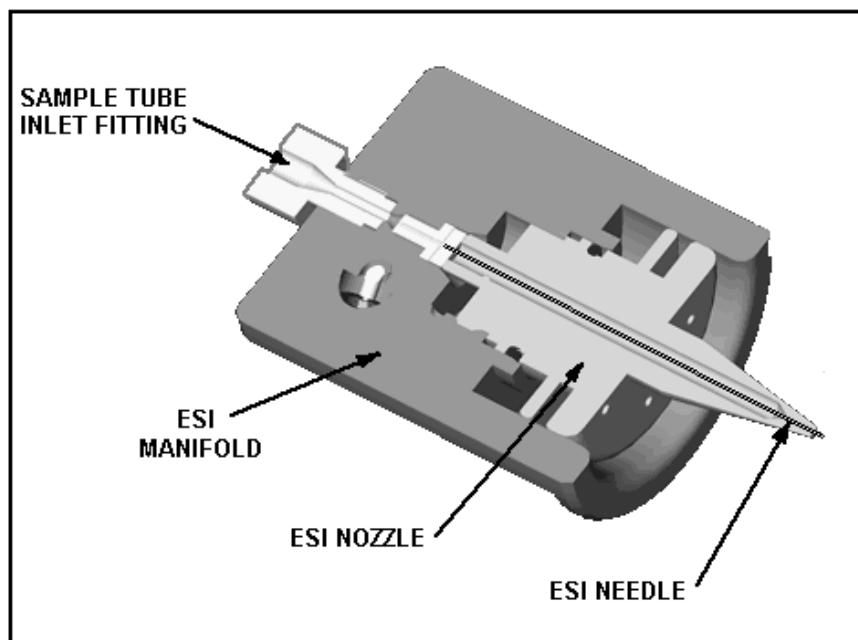


Figure 2-11. Cross sectional view of the ESI probe

A lever on the bottom of the ESI source housing allows you to adjust the angle of the ESI probe between off-axis (orthogonal) and straight-on orientation in real time. Off-axis spraying affords better long-term signal stability (robustness) for some solutions containing non-volatile matrix components, mobile phase buffers, or ion-pairing reagents.

APCI Probe

The **APCI probe** ionizes the sample by atmospheric pressure chemical ionization. The APCI probe accommodates liquid flows of 100 $\mu\text{L}/\text{min}$ to 2 mL/min without splitting. See Figure 2-12. The APCI probe includes the APCI sample tube, nozzle, sheath gas and auxiliary gas plumbing, and vaporizer. See Figure 2-13. Sample and solvent enter the APCI nozzle through the **sample tube**. The sample tube is a short section of 0.15 mm ID fused silica tubing that extends from the sample inlet to 1 mm past the end of the nozzle. The **manifold** houses the APCI nozzle and includes the sheath gas and auxiliary gas plumbing. The **APCI nozzle** sprays the sample solution into a fine mist. The **sheath gas and auxiliary gas plumbing** deliver dry nitrogen gas to the nozzle. The droplets in the mist then enter the vaporizer. The **vaporizer** flash vaporizes the droplets at temperatures up to 600 °C.

Typical vaporizer temperatures are 350 to 400 °C for flow rates of 100 $\mu\text{L}/\text{min}$, 450 to 500 °C for 1 mL/min (normal APCI flow rate), and 550 to 600 °C for 2 mL/min. The sample vapor is swept toward the corona discharge needle by the flow of the sheath and auxiliary gasses.

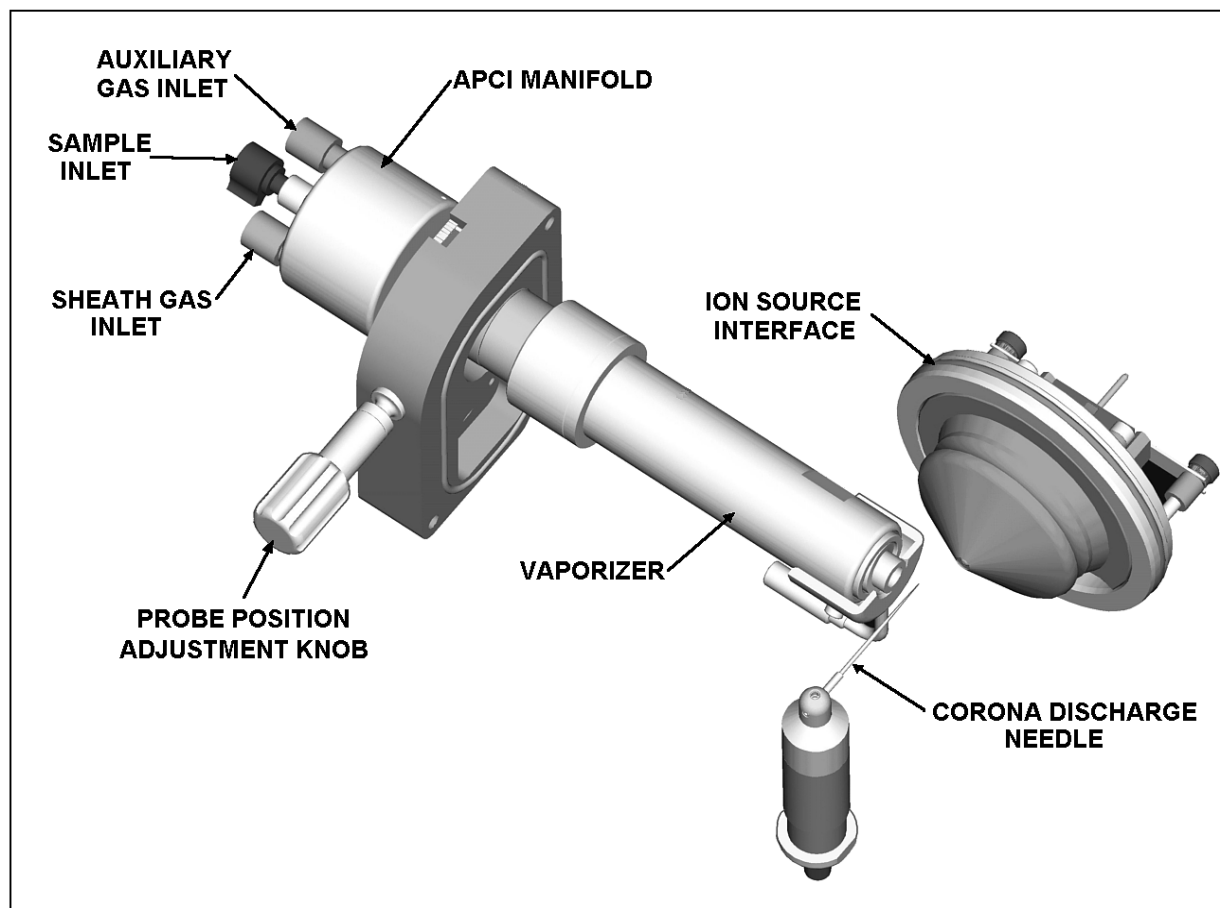


Figure 2-12. APCI probe, corona discharge needle, and ion source interface

The **corona discharge needle assembly** is mounted inside of the APCI source housing. The tip of the corona discharge needle is positioned near the vaporizer. A high potential (typically ± 3 to ± 5 kV) is applied to the **corona discharge needle** to produce a **corona discharge current** of up to 10 μA . (A typical value of the corona discharge current is 5 μA .) The corona discharge from the needle produces reagent ion plasma primarily from the solvent vapor. The sample vapor is ionized by ion-molecule reactions with the reagent ions in the plasma.

APCI requires a constant source of electrons for the ionization process. Thus, the corona discharge current is set to a specific value and regulated. The potential applied to the corona discharge needle varies, as needed, to provide the required current.

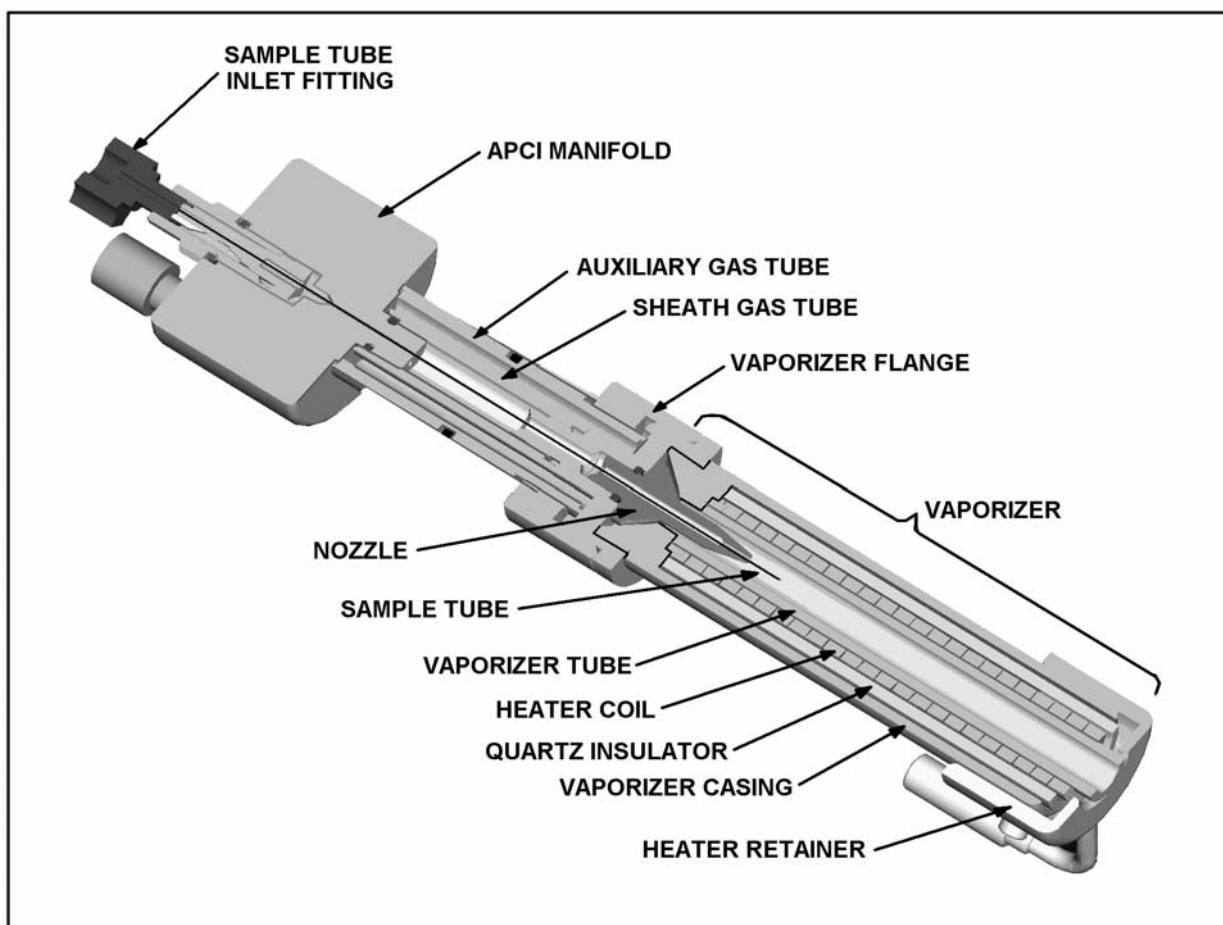


Figure 2-13. Cross sectional view of the APCI probe

Ion Source Interface

The *ion source interface* consists of the components of the API source that are held under vacuum (except for the atmospheric pressure side of the ion sweep cone). The ion source interface includes an ion transfer tube, two cartridge heaters, heater block, platinum probe sensor, vent prevent ball, and ion sweep cone. See Figure 2-14 and Figure 2-15.

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

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

The system electronics include a voltage monitor circuit and an overtemperature/undertemperature circuit to protect the heaters. The voltage monitoring circuit detects shorting failures. The overtemperature portion of the circuit is intended to function as a thermal limit switch to prevent the heater from turning on continuously above a preset temperature. The undertemperature feature identifies faults in the platinum probe sensor that would otherwise cause the heater to turn full on.

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

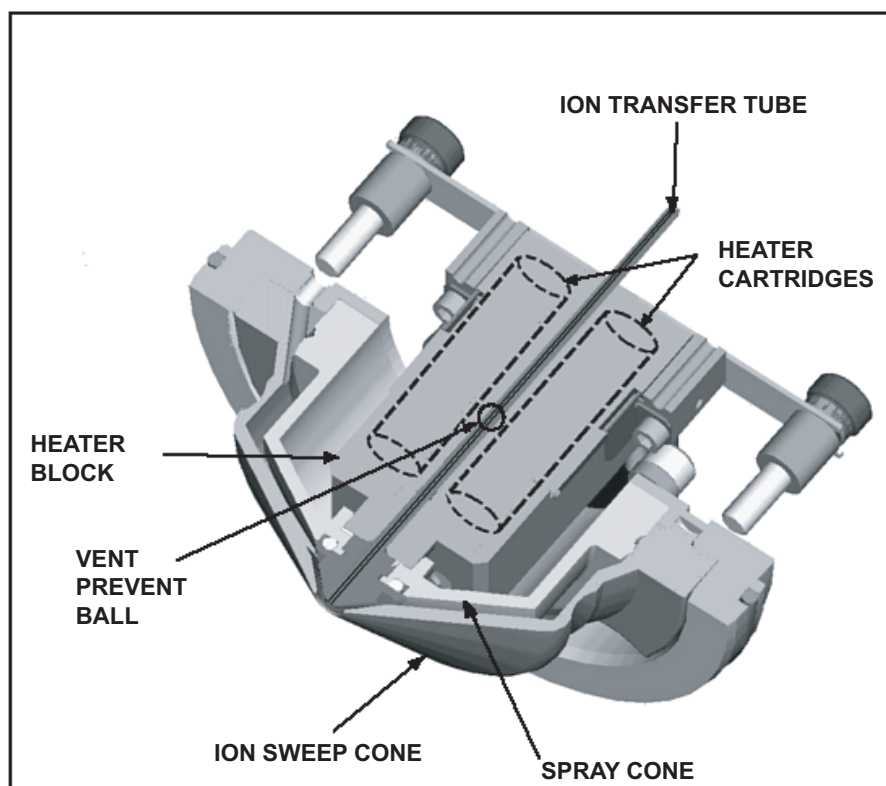


Figure 2-14. Cross sectional view of the ion source interface

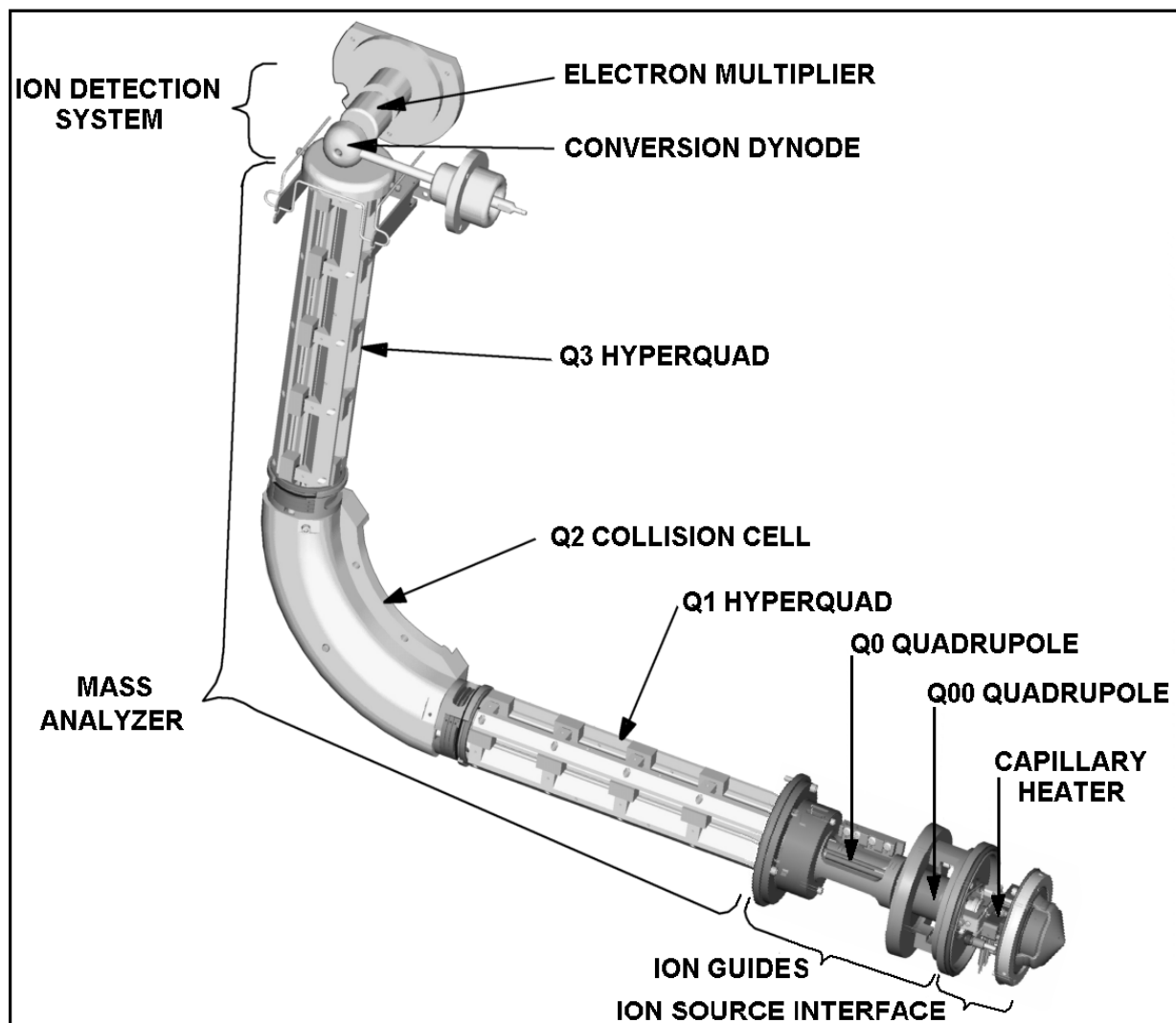


Figure 2-15. Internal (under vacuum) mass spectrometer components

Ion Guides

The *ion guides* focus the ions produced in the API source and transmit them to the mass analyzer. The TSQ Quantum system uses two ion guides:

- Q00 Ion Guide
- Q0 Ion Guide

Q00 Ion Guide

The *Q00 ion guide* is the ion guide that is located closest to the API source (Figure 2-15). The Q00 ion guide includes the tube lens, skimmer, Q00 quadrupole, interstage disk, and lens L0. See Figure 2-16.

Ions from the ion transfer tube enter the *tube lens*. The tube lens has a mass dependent potential applied to it to focus the ions towards the opening of the skimmer. An additional potential of between 0 and ± 250 V (positive for positive ions and negative for negative ions), called the *tube lens offset voltage*, can be applied to the tube lens to accelerate the ions into 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 increases sensitivity. If the tube lens offset voltage is too high, however, collisions with the background gas can be energetic enough to cause the ions to fragment. This fragmentation, called *ion source collision induced dissociation* (CID), decreases sensitivity. When you tune the TSQ Quantum instrument, you adjust the tube lens offset voltage to maximize sensitivity by balancing desolvation with fragmentation.

Ions from the tube lens pass through the skimmer and move toward the Q00 quadrupole. The *skimmer* acts as a vacuum baffle between the higher pressure ion source interface region (at 1.5 Torr) and the lower pressure Q00 ion guide region (at 50 mTorr) of the vacuum manifold. The 1.7 mm aperture of the skimmer is offset with respect to the bore of the ion transfer tube by 1.2 mm. This arrangement reduces the number of large, charged particles that pass through the skimmer and into the mass analyzer, thereby reducing detector noise. The tube lens and skimmer mount to the *interstage disk*.

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

The *lens L0* is a metal cylinder with a small hole in one end through which the ion beam can pass. A potential of between 0 and ± 3 V (negative for positive ions and positive for negative ions) is applied to lens L0 to aid in ion

transmission. Lens L0 also acts as a vacuum baffle between the Q00 and Q0 ion gauge chambers. The Q00 ion guide chamber of the vacuum manifold is evacuated to a pressure of 50 mTorr by the third inlet in the molecular drag section of the turbomolecular pump.

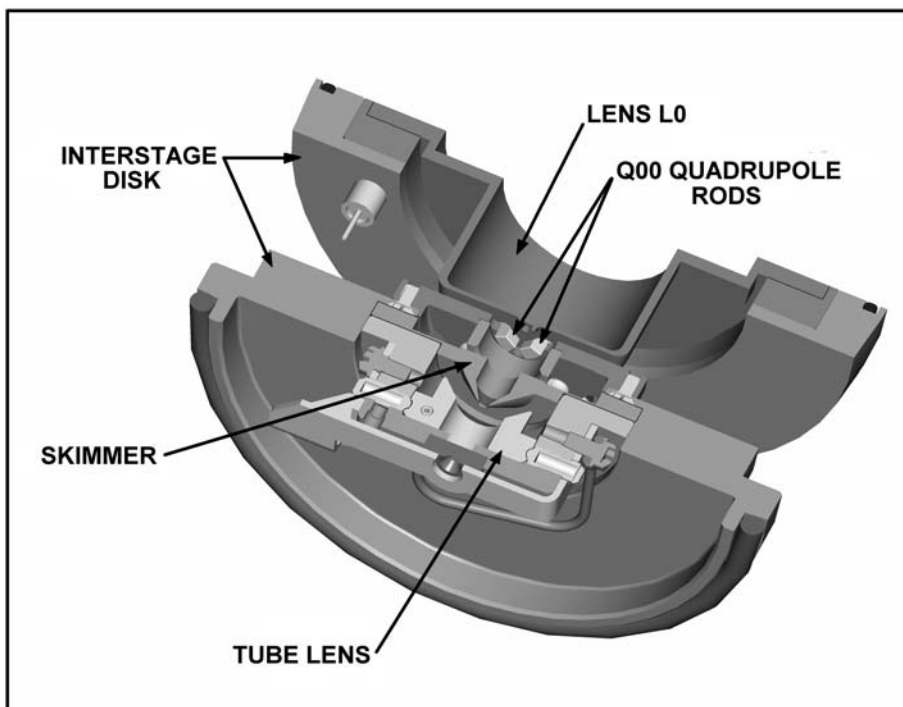


Figure 2-16. Cross sectional view of the Q00 ion guide

Q0 Ion Guide

The *Q0 ion guide* transmits ions from the Q00 ion guide to the mass analyzer. The Q0 ion guide includes the Q0 quadrupole, lenses L11 and L12, mounting cage, baffle cap, and spring. See Figure 2-17.

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

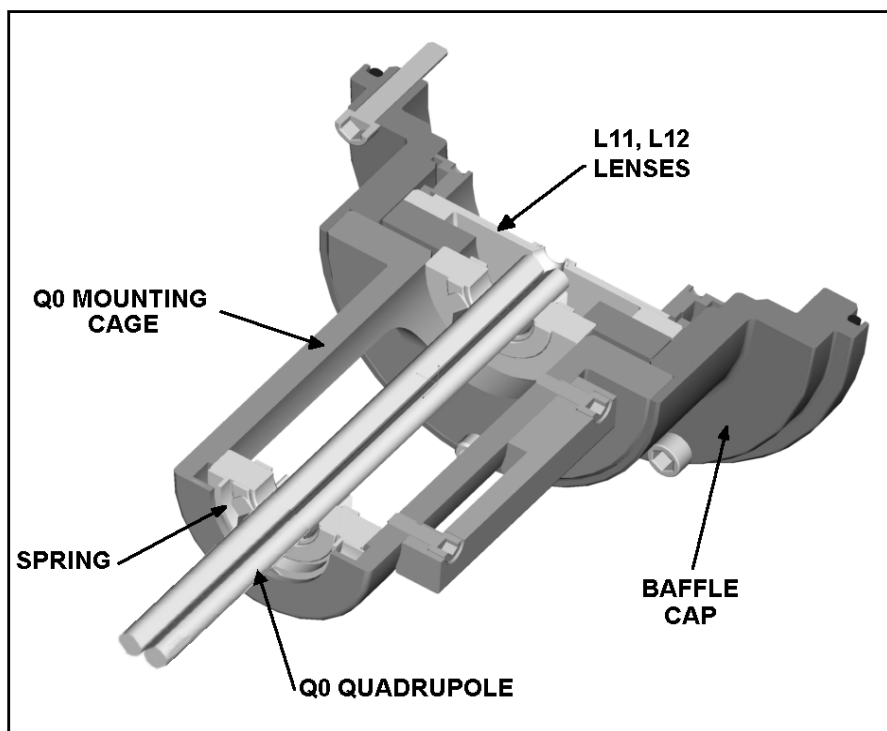


Figure 2-17. Cross-sectional view of the Q0 ion guide

The Q0 offset voltage can also be used to fragment ions. In *ion source collision-induced dissociation*, the offset voltage (typically -30 V to $+30$ V) is set to impart enough kinetic energy to the ions so that, when they collide with solvent or air molecules, the ions dissociate to form product ions. The translational kinetic energy imparted to the ions determines the degree of dissociation. At low energies, adduct ions convert to sample ions by collision-induced dissociation without fragmenting. At higher energies, molecular ions can fragment and thereby enable primitive MS/MS/MS analysis.

Q0 is held in place in a mounting cage by a spring. The mounting cage attaches to the baffle cap.

The *L11* and *L12* lenses are metal disks with a circular hole in the center through which the ion beam can pass. Together they act as a two-element cone lens. An electrical potential can be applied to the lens to accelerate (or decelerate) ions as they approach the lens and to focus the ion beam as it passes through the lens. The value ranges between 0 and ± 300 V. Lenses L11 and L22 also act as a vacuum baffle between the Q0 ion guide chamber and the mass analyzer chamber. The Q0 ion guide chamber is evacuated to a pressure of about 1 mTorr by the interstage inlet of the turbomolecular pump.

Mass Analyzer

The *mass analyzer* separates ions according to their mass-to-charge ratio and then passes them to the ion detection system. The mass analyzer on the TSQ consists of three quadrupole rod assemblies (Q1, Q2, and Q3) and three lens sets. See Figure 2-18.

The mass analyzer is described in detail in the following topics:

- Quadrupole Rod Assemblies
- RF and DC Fields Applied to the Quadrupoles
- Mass Analysis
- Collision Cell and CID Efficiency
- Quadrupole Offset Voltage
- Mass Analyzer Lenses

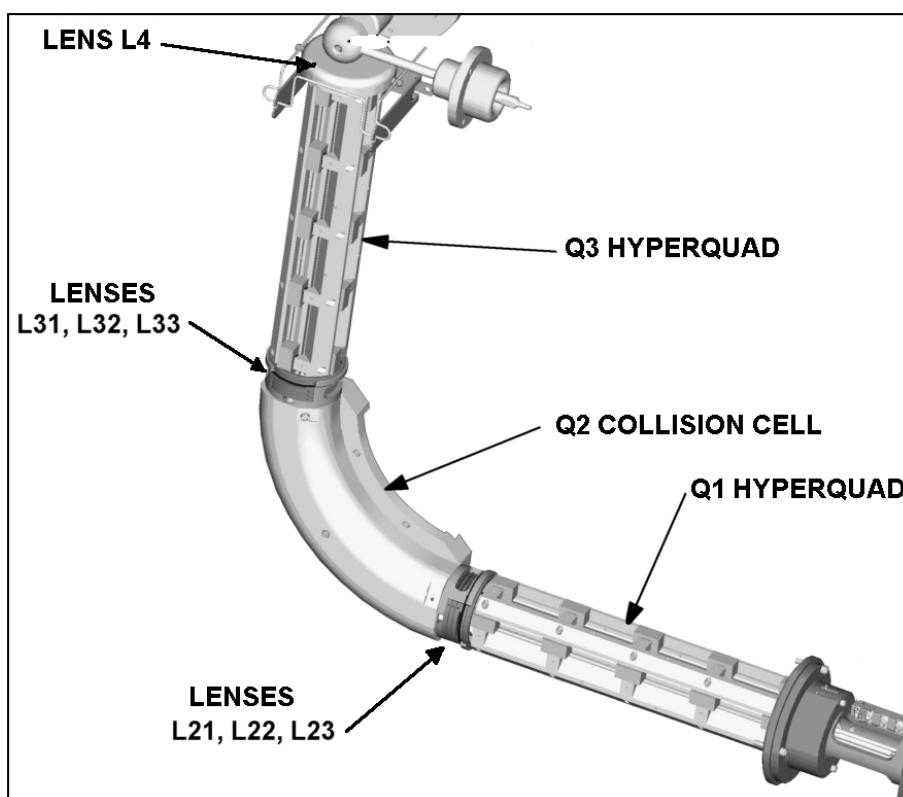


Figure 2-18. Mass analyzer

Quadrupole Rod Assemblies

The three rod assemblies used in the TSQ Quantum instrument are numbered from the ion source end of the manifold and are designated Q1, Q2, and Q3. Q1 and Q3 are true hyperbolic quadrupoles—or “hyperquads”—that enable high-resolution scans without signal loss. The hyperquad rods are 250 mm long and the field radius (the distance from the surface of the rods to the z axis) is 6 mm. See Figure 2-19. Quartz spacers act as electrical insulators between adjacent rods.

Q2 is a square-profile quadrupole rod assembly. Q2 always acts as an ion transmission device. The Q2 quadrupole rods are bent through a 90-degree arc. In addition to reducing the footprint of the instrument, this prevents the transmission of unwanted neutral species to the detector and dramatically lowers the noise level in the data. Q2 has become synonymous with the term *collision cell*. Technically, the collision cell is the chamber that encloses Q2 where collision-induced dissociation can take place if the argon collision gas is present. See Figure 2-20.

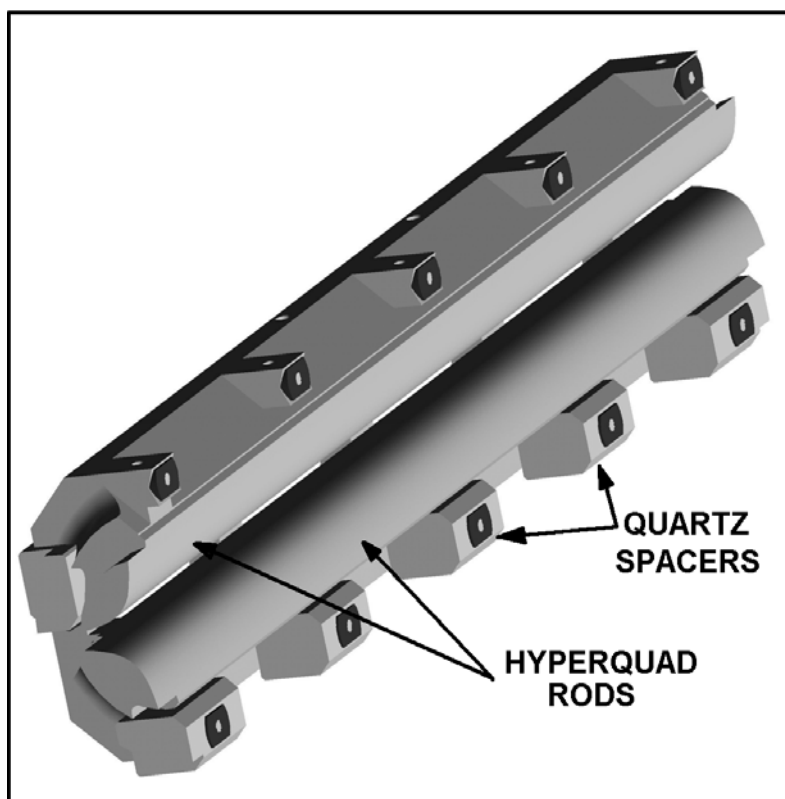


Figure 2-19. Cross sectional view of the Q1 or Q3 hyperquad

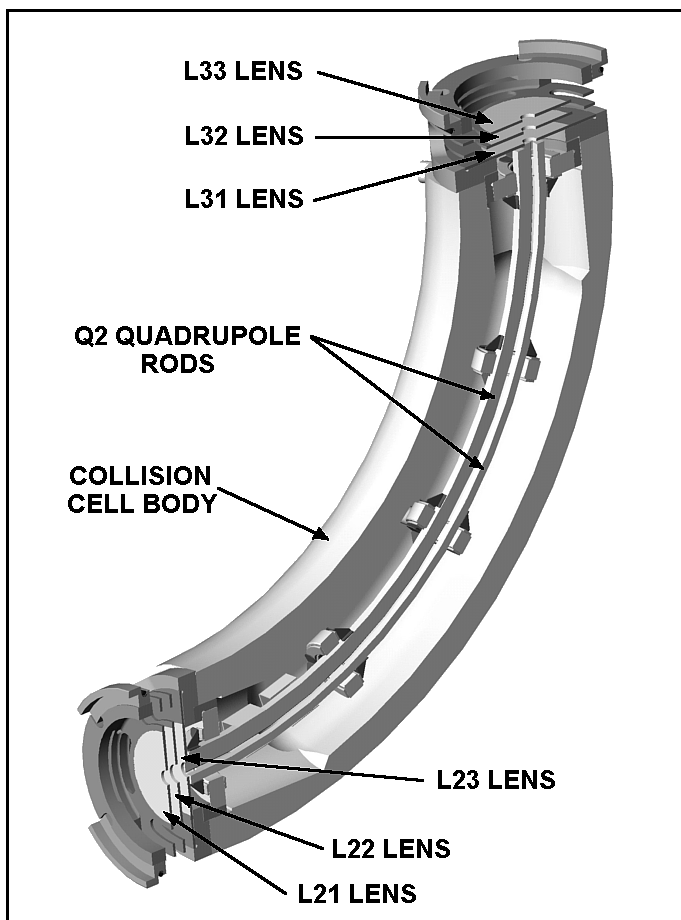


Figure 2-20. Cross-sectional view of the Q2 square quadrupole and collision cell

RF and DC Fields Applied to the Quadrupoles

In a quadrupole rod assembly, rods opposite each other in the array are connected electrically. Thus, the four rods can be considered to be two pairs of two rods each. Ac and dc voltages are applied to the rods and these voltages are ramped during the scan. Voltages of the same amplitude and sign are applied to the rods of each pair. However, the voltages applied to the different rod pairs are equal in amplitude but opposite in sign. See Figure 2-21.

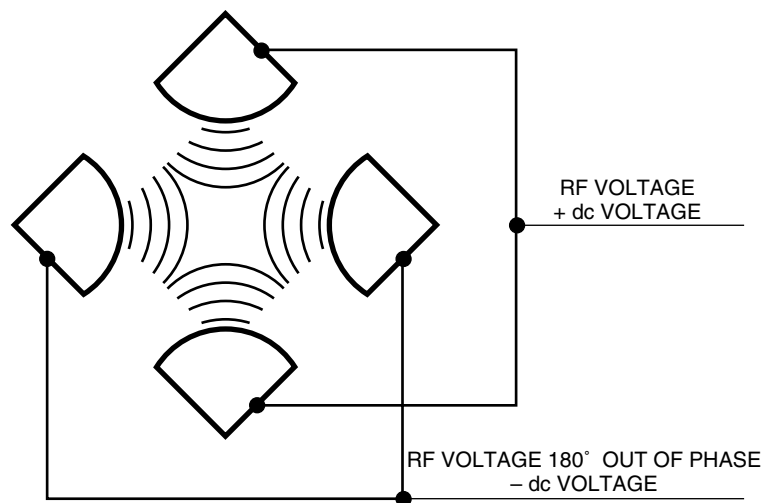


Figure 2-21. Polarity of the RF and dc voltages applied to the rods of the Q1 and Q3 mass analyzers. Voltages of the same amplitude and sign are applied to each rod pair. However, the voltages applied to the other rod pair are equal in amplitude but opposite in sign.

The ac voltage applied to the quadrupole rods is of constant frequency (1.123 MHz) and of variable amplitude (0 to 10000 V peak-to-peak). Because the frequency of this ac voltage is in the radio frequency range, it is referred to as **RF voltage**. The dc voltage applied to the rods can vary from 0 to ± 840 V. See Figure 2-22. The ratio of RF voltage to dc voltage determines the ability of the mass spectrometer to separate ions of different mass-to-charge ratios.

The first and third quadrupole rod assemblies (Q1 and Q3 hyperquads) can act as mass analyzers or as ion transmission devices. When both RF and dc voltages are applied, Q1 and Q3 function as mass analyzers. When only RF voltage is applied, they act as ion transmission devices. In the ion transmission mode, the quadrupole rod assemblies allow ions in a wide window of mass-to-charge ratios to pass.

The square quadrupole rod assembly (Q2) operates in the ion transmission mode only. Surrounding Q2 is a collision cell where collision-induced dissociation (CID) can take place if the argon collision gas is present in the cell.

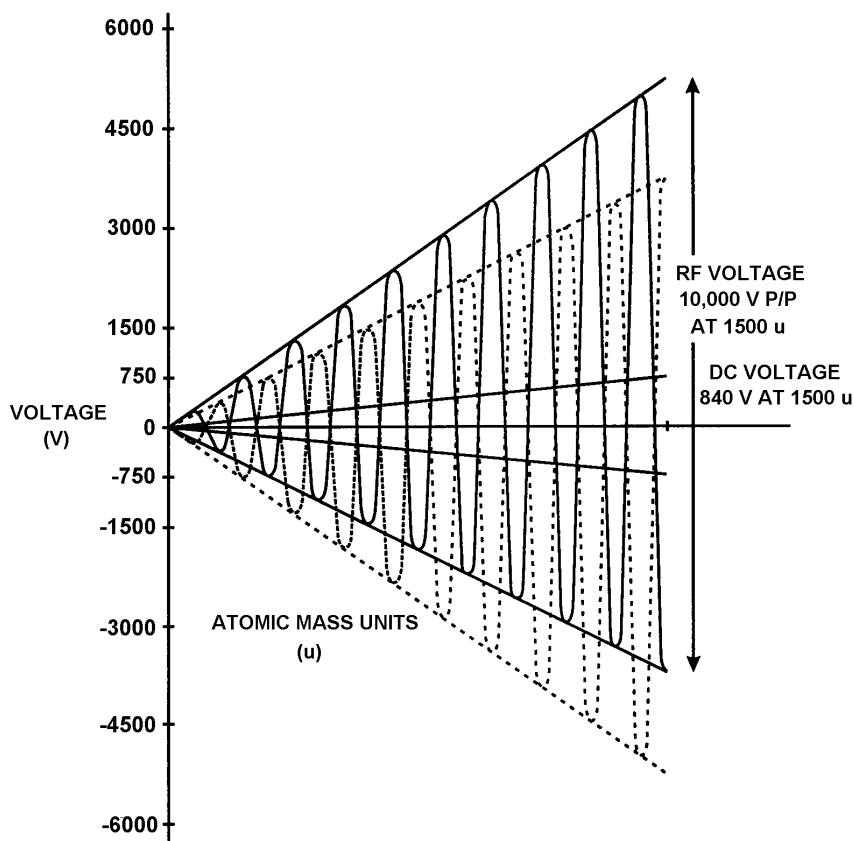


Figure 2-22. Magnitude of the RF and dc voltages applied to the rods of the Q1 and Q3 mass analyzers. The RF voltage applied to the rods varies from 0 to 10000 V P/P, and the dc voltage varies from 0 to ± 840 V. The solid line represents the combined RF and dc voltage applied to one rod pair, and the dashed line represents the combined RF and dc voltage applied to the other rod pair.

Mass Analysis

The *mass analyzers* (Q1 and Q3) are square arrays of precision-machined and precision-aligned hyperbolic rods. The rods are charged with a variable ratio of RF voltage and dc voltage (Figure 2-22). These potentials give rise to an electrostatic field that gives stable oscillations to ions with a specific mass-to-charge ratio and unstable oscillations to all others.

At any given instant, one particular set of RF and dc voltage values is being applied to the mass analyzer rods. Under these conditions, only ions of one mass-to-charge ratio (for example, m/z 180) are maintained within bounded oscillations as their velocity carries them through the mass analyzer. During this same time, all other ions undergo unbounded oscillations. (These ions strike one of the rod surfaces or are ejected from the rod assembly, become neutralized, and are pumped away.)

Then, at a later time, both RF and dc voltages change, and ions of the next mass-to-charge ratio (for example, m/z 181) are allowed to pass, while all other ions (including m/z 180) become unstable and undergo unbounded oscillations. This process continues, with ions of one mass-to-charge ratio after another being transmitted, as the RF and dc voltages change in value. At the end of the scan, the RF and dc voltages are discharged to zero, and the process is repeated.

The potentials on the quadrupole rods can be changed rapidly and precisely. The RF and dc voltages in the TSQ Quantum instrument can be scanned over the full mass range of the system (for example, m/z 30 to 1500) in as short a time as 0.1 s. (Although, under the conditions usually employed in mass analysis, such a scan would normally be done in about 2 s.)

The more closely the electrostatic field generated by a set of quadrupole rods approximates a hyperbolic geometry, the better their operating characteristics will be. Thus, the precision hyperbolic quadrupole rods of the TSQ Quantum instrument provide excellent sensitivity, peak shape, resolution, and high mass transmission.

Collision Cell and CID Efficiency

The *collision cell quadrupole rod assembly* (Q2), which always acts as an ion transmission device, is a quadrupole array of square-profile rods. The rods are charged with a variable RF voltage. This RF voltage gives rise to an electrostatic field that gives stable oscillations to ions in a wide window of mass-to-charge ratios.

The collision cell curves through 90° (Figure 2-20). The curve in the Q2 rod assembly has no effect on the transmission of ions through it. However, fast neutral particles (and photons) do not negotiate the curve. They exit from the rod assembly and are pumped away. Therefore, the net effect of the curve in Q2 is a dramatic lowering of noise due to neutral particles (and photons).

In the MS/MS scan modes, the collision cell is emptied of ions in between scans by applying a large voltage of opposite polarity to the rod pairs. This ensures that no ions remain in the collision cell from scan to scan.

Surrounding Q2 is the **collision cell**. The collision cell is usually pressurized from about 1 to 4×10^{-3} Torr with argon **collision gas**. The collision cell is the site where **collision-induced dissociation (CID)** takes place.

CID is a process in which an ion collides with a neutral atom or molecule and then, because of the collision, dissociates into smaller fragments. The mechanism of dissociation involves the conversion of some of the translational kinetic energy (TKE) of the ion into internal energy such that the ion is placed in an excited state. If the internal energy is sufficient, the ion fragments.

The efficiency of the CID process can be stated in three expressions:

- collection efficiency
- fragmentation efficiency
- overall CID efficiency

The **collection efficiency** is the ratio of the ion flux at the exit of the collision cell to that at its entrance. With no collision gas present, virtually 100% collection efficiency is obtained. Collection efficiency is a mass-dependent parameter. For example, with a mid-range collision gas pressure, the collection efficiency might vary from about 50% for comparatively less massive ions (which are more prone to scatter) up to 75% for comparatively more massive ions (which are less prone to scatter).

The **fragmentation efficiency** is the fraction of the ion flux at the exit of the collision cell that is due to fragmented ions. Fragmentation efficiency depends directly upon the stability of the ion and indirectly upon the mass of the ion. The more stable the ion, the less likely it will be for a given collision to fragment the ion. The more massive the ion, the greater will be its ability to distribute the vibrational energy imparted to it by a collision; and therefore, the less likely it will be for the ion to fragment.

With a mid-range collision gas pressure, fragmentation efficiency might vary from 15% to 65% for various compounds. As the collision gas pressure is increased, the fragmentation efficiency for all compounds approaches 100% due to multiple collisions, but the collection efficiency decreases due to scattering.

The **overall CID efficiency** is the product of the collection efficiency and the fragmentation efficiency. The overall CID efficiency exhibits a maximum at some intermediate pressure. This is true because, as the pressure is increased beyond the optimum value, more and more collisions take place, the probability of scattering increases, and fewer and fewer ions pass through the collision cell. Thus, the collection efficiency decreases. And, as the pressure is decreased from its optimum value, fewer and fewer collisions take place. Thus, the fragmentation efficiency decreases.

Quadrupole Offset Voltage

The *quadrupole offset voltage* is a dc potential applied to the quadrupole rods in addition to the ramping dc voltage. The offset voltage applied to the two rod pairs of the assemblies are equal in amplitude and equal in sign. The purpose of the quadrupole offset voltage is to accelerate or decelerate ions and, thus, to set the translational kinetic energy (TKE) of the ions as they enter the quadrupole rod assembly.

In general, the offset voltages applied to Q1 and Q2 are fixed for a given experiment. However, in MS/MS experiments, the quadrupole offset voltage applied to Q3 usually varies as a scan proceeds. The TSQ Quantum system automatically computes the Q3 quadrupole offset voltage necessary for a given experiment and then varies the voltage, as appropriate, as each scan proceeds.

The offset voltage applied to Q2 (which contains the collision cell) is called the *collision energy*. The collision energy is the difference in potential between the API source (where parent ions are formed) and Q2 (where they collide with collision gas). As the offset voltage on Q2 is increased, the TKE of the parent ions is also increased. Thus, increases in the Q2 offset voltage increase the energy of ion / molecule collisions. The collision energy is generally set to one value for an entire scan and can be set from 0 to ± 200 V.

Before any mass spectra are obtained, Q1 is tuned in the Q1MS scan mode (Q2 and Q3 RF voltage only), and Q3 is tuned in the Q3MS scan mode (Q1 and Q2 RF voltage only). During tuning, the optimum quadrupole offset voltage is determined for Q1 and for Q3.

Mass Analyzer Lenses

The TSQ Quantum mass analyzer has three lens sets. See Figure 2-18 on page 2-24. Those between Q1 and Q2 are designated L21, L22, L23; those between Q2 and Q3 are designated L31, L32, L33; and the lens between Q3 and the ion detection system is designated as L4 (or exit lens). All of the lenses have circular holes in their centers through which the ion beam passes.

The lens assemblies are also used to retain the three rod assemblies. This allows the lenses and rod assemblies to be axially aligned accurately and automatically.

The *L2x lens set* (between Q1 and Q2) and the *L3x lens set* (between Q2 and Q3) serve three functions. Their first function is to minimize the amount of collision gas that enters the mass analyzers (Q1 and Q3) from the collision cell (Q2). (For high-mass transmission, it is important to maintain a low pressure in the mass analyzers.) Lenses L23 and L31 form two of the walls of the collision cell, thus they tend to hold the collision gas in the collision cell. However, each of these lenses necessarily has a hole in it through which the ion beam passes. Collision gas escapes through these holes. Lenses L22 and

L21 on one side of Q2 and lenses L32 and L33 on the other side act as baffles that help to prevent the gas that escapes from the collision cell from entering the mass analyzers.

The second function of the L2x and L3x lens sets is to shield Q1 from the RF voltage applied to Q2 and vice versa (L2x lens set) and to shield Q3 from the RF voltage applied to Q2 and vice versa (L3x lens set).

The third function of the L2x and L3x lens sets is to focus the ion beam. The three lenses between Q1 and Q2 (and those between Q2 and Q3) together form a three-element aperture lens. The first and third lenses are generally set to similar or identical values and the central lens is set to a value different (either higher or lower) from the other two.

The voltage applied to each of the lenses can vary from about -300 to +300 V. Typically, however, the voltage applied to the first and third elements of the L2x lens set is somewhat greater than the quadrupole offset voltage applied to Q1. Because the Q1 quadrupole offset voltage is generally set to about ± 5 V (depending on the charge of the ions of interest), the voltage applied to lenses L21 and L23 is typically about -10 V for positive ions and +10 V for negative ions. The voltage applied to the central lens of the L2x lens set is typically about ± 100 V.

In the Q3MS scan mode, the voltage applied to the lenses of the L3x lens set is about the same as that applied to the corresponding lens in the L2x lens set. Note, however, that in the MS/MS scan modes, the voltage applied to the L3x lens set automatically varies with the quadrupole offset voltage applied to Q3. As the Q3 quadrupole offset voltage ramps, the voltages applied to the lenses ramp correspondingly.

Lens L4 is located between Q3 and the ion detection system. L4 is held at ground potential. Its purpose is to shield Q3 from the high voltage applied to the ion detection system and to shield the ion detection system from the high RF voltages applied to Q3.

Ion Detection System

The TSQ Quantum mass spectrometer is equipped with a high sensitivity, off-axis **ion detection system** that produces a high signal-to-noise ratio and allows for voltage polarity switching between positive ion and negative ion modes of operation. The ion detection system includes a 15-kV conversion dynode and a channel electron multiplier. The ion detection system is located at the rear of the vacuum manifold behind the mass analyzer. See Figure 2-23.

The **conversion dynode** is a concave metal surface that is located at a right angle to the ion beam. A potential of +15 kV for negative ion detection or -15 kV for positive ion detection is applied to the conversion dynode. When an ion strikes the surface of the conversion dynode, one or more secondary particles are produced. These secondary particles can include positive ions, negative ions, electrons, and neutrals. When positive ions strike a negatively charged conversion dynode, the secondary particles of interest are negative

ions and electrons. When negative ions strike a positively charged conversion dynode, the secondary particles of interest are positive ions. These secondary particles are focused by the curved surface of the conversion dynode and are accelerated by a voltage gradient into the electron multiplier.

The **electron multiplier** includes a cathode and an anode. The **cathode** of the electron multiplier is a lead-oxide, funnel-like resistor. See Figure 2-23. A potential of up to -2.5 kV is applied to the cathode by the **high voltage ring**. The exit end of the cathode (at the anode) is near ground potential. The cathode is held in place by the high voltage ring, two **support plates**, the **electron multiplier support**, and the **electron multiplier shield**. A spring washer applies a force to the cathode to hold it in contact with the electron multiplier shield. The electron multiplier support is attached to a base plate that is mounted to the vacuum manifold by three screws.

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

Secondary particles from the conversion dynode strike the inner walls of the electron multiplier cathode with sufficient energy to eject electrons. The ejected electrons are accelerated farther into the cathode, drawn by the increasingly positive potential gradient. Due to the funnel shape of the cathode, the ejected electrons do not travel far before they again strike the inner surface of the cathode, thereby causing the emission of more electrons. Thus, a cascade of electrons is created that finally results in a measurable current at the end of the cathode where the electrons are collected by the anode. The current collected by the anode is proportional to the number of secondary particles striking the cathode. Typically, the electron multiplier is set to a gain of about 3×10^5 (that is, for each ion or electron that enters, 3×10^5 electrons exit) in MS mode and 2×10^6 in MS/MS mode. The current that leaves the electron multiplier via the anode is converted to a voltage by the electrometer circuit and recorded by the data system. Refer to the topic **Ion Detection System Electronic Assemblies** on page 2-52.

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

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

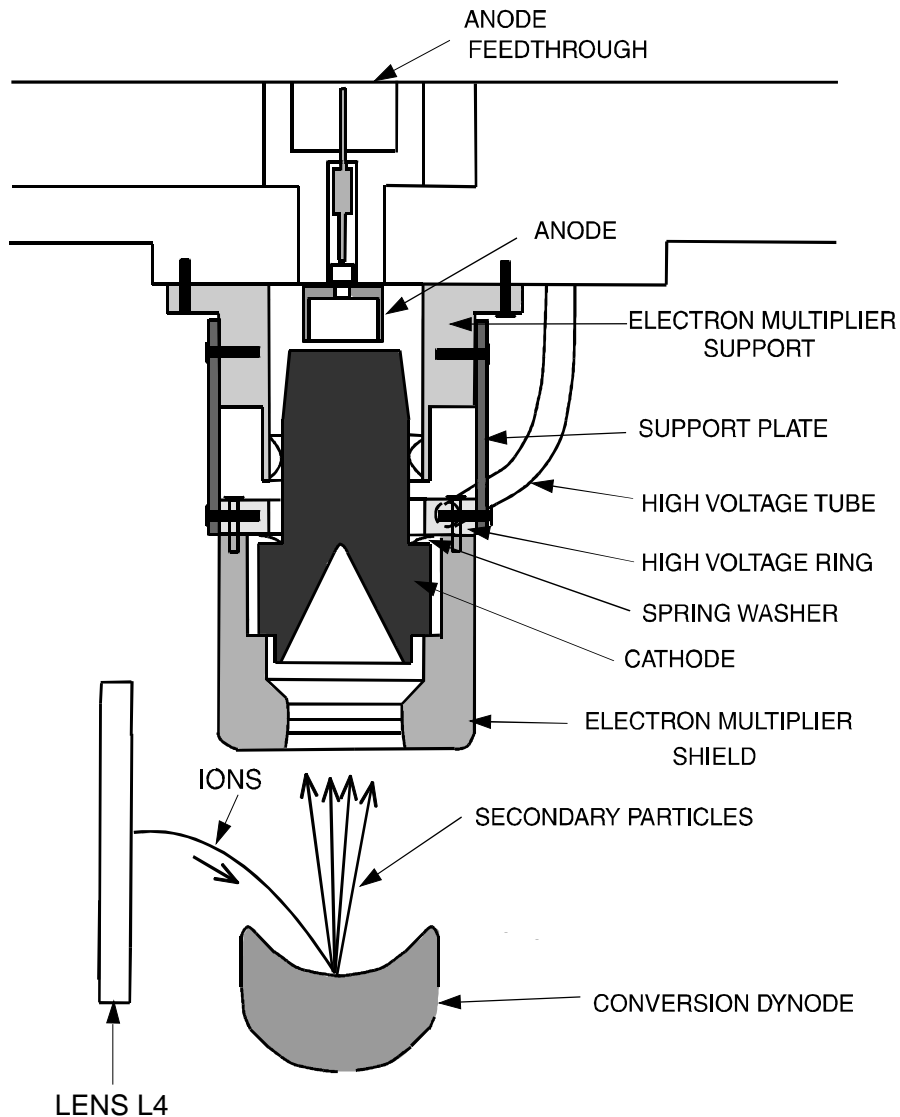


Figure 2-23. Cross sectional view of the ion detection system, showing the electron multiplier and the conversion dynode

Vacuum System and Inlet Gasses Hardware

The ***vacuum system*** evacuates the region around the ion source interface, ion guides, mass analyzer, and ion detection system. The principal components of the vacuum system include the following:

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

The ***inlet gasses hardware*** controls the flow of collision gas, sheath gas, auxiliary gas, and air (during venting) into the mass spectrometer. The inlet gasses hardware includes the following components:

- Vent Valve
- Collision Gas Flow Control Valves
- Sheath Gas Valve
- Auxiliary Gas Valve

A functional block diagram of the vacuum system and inlet gasses hardware is shown in Figure 2-24.

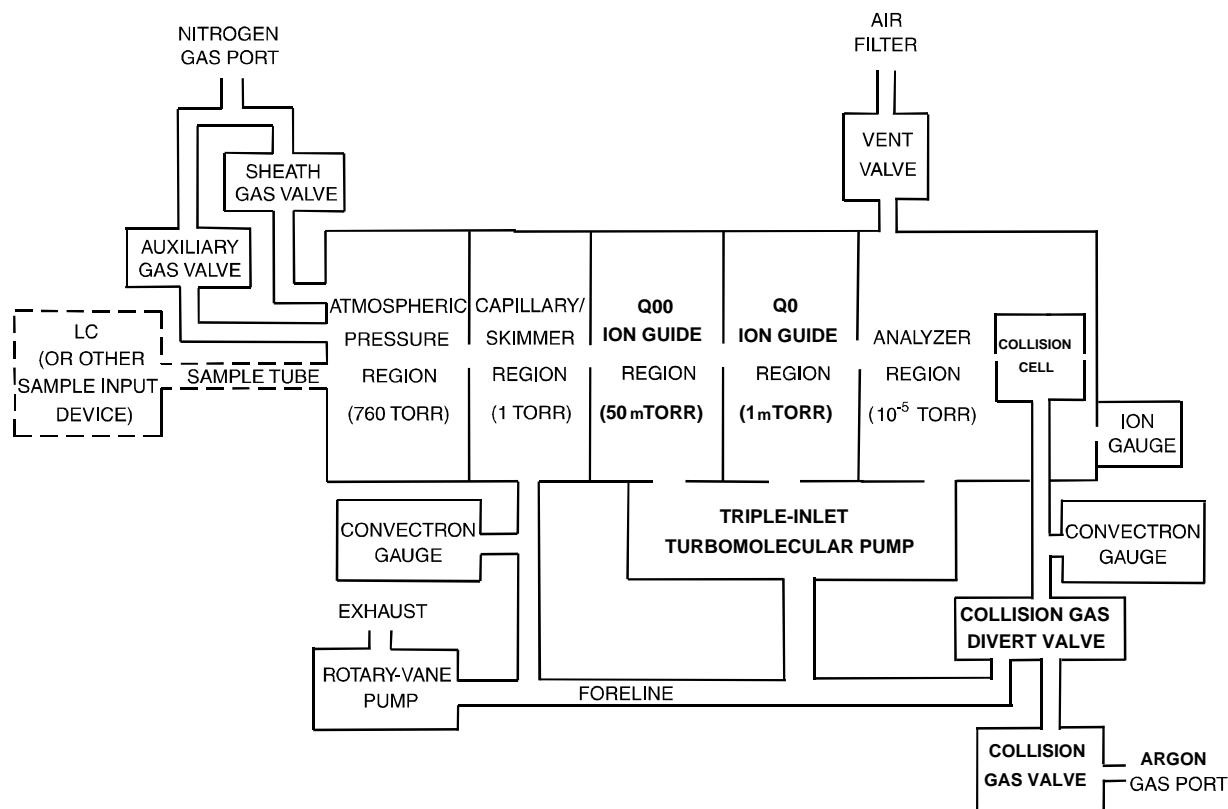


Figure 2-24. Functional block diagram of the vacuum system and inlet gasses hardware

Vacuum Manifold

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

The vacuum manifold is divided into four chambers by three baffles. See Figure 2-25. The region inside the first chamber, called the *ion transfer tube-skimmer region*, is evacuated to 1 Torr by the forepump. The region inside the second chamber, called the *Q00 ion guide region*, is evacuated to 50 mTorr by the third inlet in the molecular drag section of the triple-inlet turbomolecular vacuum pump. The region inside the third chamber, called the *Q0 ion guide region*, is evacuated to 1 mTorr by the interstage port of the turbomolecular vacuum pump. The region inside the fourth chamber, called the *analyzer region*, is evacuated to less than 10^{-5} Torr by the high vacuum port of the turbomolecular pump. The turbomolecular pump in turn discharges into the forepump through the foreline.

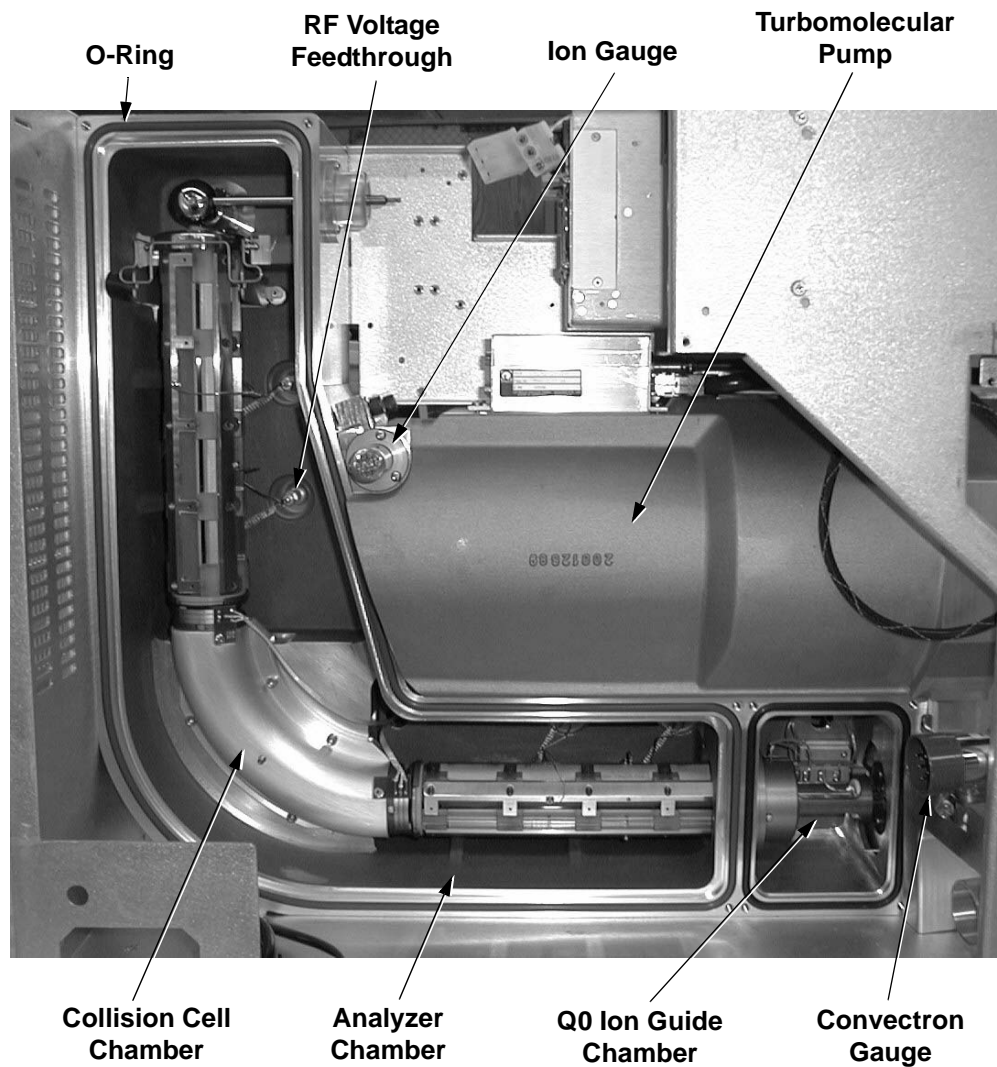


Figure 2-25. Vacuum manifold (interior)

The collision cell chamber, inside the analyzer chamber, has a user controlled argon pressure of between 1 and 4 mTorr when CID is turned on. Argon in the collision cell is evacuated by the forepump when CID is turned off.

The vacuum manifold has the following feedthroughs and inlets:

- A feedthrough for the high voltage for the conversion dynode
- A feedthrough for the high voltage for the electron multiplier
- A feedthrough for the ion current signal from the anode of the electron multiplier
- Two feedthroughs for the Q1 hyperquad RF voltage
- Two feedthroughs for the Q3 hyperquad RF voltage
- A feedthrough for the Q2 quadrupole RF voltage
- A feedthrough for lens L21, L22, L23, L31, L32, and L33 voltages
- A feedthrough for lens L0, L11, and L12 voltages
- A feedthrough for the Q00 and Q0 ion guide RF voltages
- A feedthrough for the tube lens offset voltage, ion transfer tube offset voltage, and ion transfer tube heater voltages
- A vacuum connection for measuring the pressure in the analyzer region with the ion gauge
- An argon gas inlet into the collision cell
- A vent gas inlet

Two removable *side cover plates* on the left side of the vacuum manifold allow access to the Q0 ion guide, mass analyzer, and ion detection system. Two electrically conductive O-rings provide a vacuum-tight seal between the side cover plates and the vacuum manifold.

Turbomolecular Pump

A Leybold TW220/150/15S triple-inlet *turbomolecular pump* provides the vacuum for the Q00 ion guide region, Q0 ion guide region, and analyzer region of the vacuum manifold. The turbomolecular pump mounts onto the top of the vacuum manifold (Figure 2-25).

The turbomolecular pump has three pumping inlets:

- A high-vacuum inlet at the top of the rotor stack, which evacuates the analyzer chamber
- An interstage inlet about halfway down the rotor stack, which evacuates the Q0 ion guide chamber immediately in front of the first mass analyzer, Q1
- A third inlet in the molecular drag section of the pump, which evacuates the Q00 ion guide chamber

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

Power to the turbomolecular pump is shut off if the foreline pressure, as measured by the Convectron gauge, is too high, or if the turbomolecular temperature is too high. Vacuum protection is discussed further in the topic **Vacuum System Electronic Assemblies** on page 2-48.

Forepump

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

The forepump is connected to the turbomolecular pump by a section of 3.8 cm (1.5 in.) ID reinforced PVC tubing. The power cord of the forepump is plugged into the outlet labeled *Forepump* on the power panel (see Figure 2-7 on page 2-11). This outlet supplies power to the pump and is controlled by the vacuum service switch and the main power circuit breaker switch, but not by the electronics service switch.

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

Convectron Gauges

A *Convectron*[®] *gauge* measures the pressure in the ion transfer tube-skimmer region of the vacuum manifold and the foreline, which connects the turbomolecular pump and the forepump. A second Convectron gauge measures the pressure of argon collision gas in the collision cell.

The Convectron gauge uses a Wheatstone bridge with a temperature dependent resistor to measure pressure down to a fraction of a millitorr. The voltage present at the top of the bridge depends on how fast the resistor can radiate heat, which is related to the pressure. The pressure measured by the Convectron gauge is monitored by vacuum protection circuitry on the Source PCB, which in turn is monitored by the embedded computer on the System Control PCB. The vacuum protection circuitry detects whether the foreline pressure is too high for the proper operation of the turbomolecular pump.

Ion Gauge

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

Vent Valve

The *vent valve* allows the vacuum manifold to be vented to air that has been filtered through a sintered nylon filter. The vent valve is a solenoid-operated valve. The vent valve is controlled by the Vent Delay PCB. The vent valve is closed when the solenoid is energized. If the power fails or the vacuum service switch is placed in the Service Mode position or the main power circuit breaker is placed in the Off (O) position, a 4-farad capacitor located in the Power Entry Module keeps the solenoid in the closed position for several minutes. If power is not restored in this time, then the solenoid opens and the system is allowed to filtered air. The vent valve closes after power is restored to the mass spectrometer. The vent valve is located in the area of Q2.

Collision Gas Flow Control Valves

The *collision gas flow control valves* control the flow of argon collision gas into and out of the Q2 collision cell. A solenoid valve acts to shut off argon gas flow valve to the cell. The collision gas pressure is regulated by a proportional valve that is controlled by the data system. You can set the collision gas pressure (0 to 4 mTorr) in the Define Scan view from the Tune Master window.

Ions entering the Q2 collision cell collide with the argon collision gas, and then, because of the collision, dissociates into smaller fragments. Refer to the topic **Collision Cell and CID Efficiency** on page 2-29.

Argon enters the mass spectrometer through a 1/8-in. port on the left side of the mass spectrometer. See Figure 2-26.

A second proportional valve allows the forepump to evacuate the Q2 collision cell of argon and “waste” gasses when CID is turned off. The TSQ Quantum system automatically opens and closes the collision gas evacuation valve depending upon whether Q2 is acting as an ion transmission device or a collision cell.

Sheath Gas Valve

The *sheath gas valve* controls the flow of sheath gas (nitrogen) into the API source. Dry nitrogen (690 ± 140 kPa [100 ± 20 psi], 99% purity) enters the mass spectrometer through a 1/4-in. port on the left side of the mass spectrometer. See Figure 2-26. A solenoid shutoff valve starts and stops the flow of nitrogen to the API source. The sheath gas pressure is regulated by a valve that is controlled by the data system. You can set the sheath gas flow rate (20 to 100 in arbitrary units) in the ESI Source and APCI Source dialog boxes from the Tune Master window. The sheath gas enters the API source through 1/8-in. ID tubing.

Auxiliary Gas Valve

The *auxiliary gas valve* controls the flow of auxiliary gas (nitrogen) into the API source. Dry nitrogen (690 ± 140 kPa [100 ± 20 psi], 99% purity) enters the mass spectrometer through a 1/4-in. port on the left side of the mass spectrometer. A solenoid shutoff valve starts and stops the flow of nitrogen to the API source. The auxiliary gas pressure is regulated by a flow valve that is controlled by the data system. You can set the auxiliary gas flow rate (0 to 60 in arbitrary units) in the ESI Source and APCI Source dialog boxes. The auxiliary gas enters the API source through 1/8-in. ID tubing.

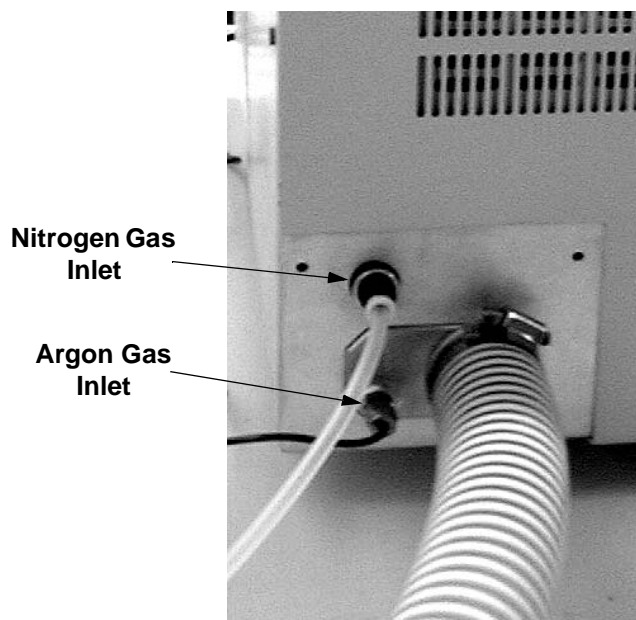


Figure 2-26. Nitrogen and argon gas inlets

Cooling Fans

Four fans provide cooling for the mass spectrometer. One pancake fan cools the turbomolecular pump. One 16-in. linear fan cools the Analyzer Control PCB, turbomolecular pump, and DC Rod Driver PCB. Two 10-in. linear fans cool the RF Amplifier PCBs and DC Rod Driver PCB. Air intake is from the front and front side panels. Air exhaust is from the rear left, rear right side panels and rear panel.

Power to the fans is provided by the +24 V power supply (PS1). Power to the fans is controlled by the vacuum service switch and the main power circuit breaker switch, but not by the electronics service switch.

Caution. To ensure proper cooling, the mass spectrometer must always be operated with its covers in place.

Electronic Assemblies

The electronic assemblies that control the operation of the mass spectrometer are distributed among various printed circuit boards (PCBs) and other modules located in the tower, embedded computer, and on or around the vacuum manifold of the mass spectrometer.

The electronic assemblies of the mass spectrometer include the following:

- Power Entry Module and Power Distributions
- System Control PCB and Embedded Computer
- Vacuum System Electronic Assemblies
- RF Voltage Generation Electronic Assemblies
- Ion Detection System Electronic Assemblies
- Analyzer Control PCB

A diagram of the electronic assemblies and their interconnection with the various components of the mass spectrometer is shown in Figure 2-27.

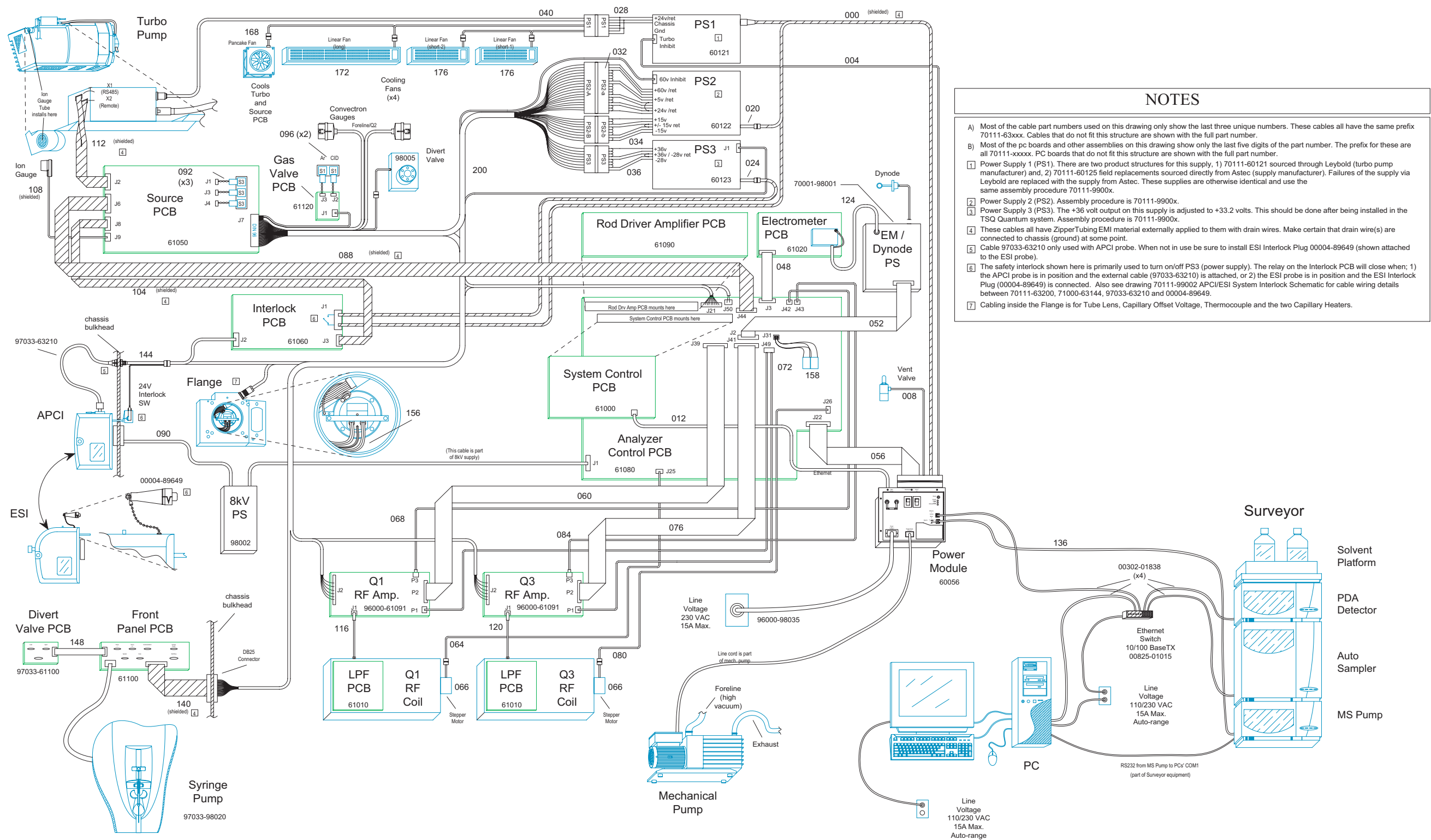


Figure 2-27. TSQ Quantum electronic interconnect diagram

Power Entry Module and Power Distribution

The **Power Entry Module** provides system power control, a contact closure interface, vent valve control, an Ethernet 100 base-T connection from the System Control PCB to the data system PC, a mechanical pump failure protection circuit (linked to vent valve control), a system reset button, status LEDs, and service ports. See Figure 2-7 on page 2-11.

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

- Main power circuit breaker switch
- Surge suppressor
- Line filter
- Electronics service switch
- Vacuum service switch

A functional block diagram of the Power Entry Module and mass spectrometer power distribution is shown in Figure 2-28.

Line power (230 V ac \pm 10%, 13 A or greater, 50/60 Hz, single phase) enters the power panel on the right side panel of the mass spectrometer, passes through the main power circuit breaker, surge suppressor, and then to a line filter (see Figure 2-7).

The **main power circuit breaker switch**, located on the right side panel of the mass spectrometer (see Figure 2-7), shuts off all power to the mass spectrometer, including the vacuum system. After the main power circuit breaker switch, power goes to the surge suppressor.

The **surge suppressor** protects the mass spectrometer from surges in the line power.

The **line filter** removes noise from the line power. After the line filter, power goes to the vacuum service switch and to the electronics service switch.

The **vacuum service switch** is a circuit breaker that allows you to turn off power to the vacuum system. In the Service Mode position the switch removes power to the forepump and the +24 V power supply (PS1). In the Operational Mode position power is supplied to the forepump and PS1.

The **+24 V power supply (PS1)** provides +24 V power to the four fans and the turbomolecular pump controller, which powers the turbomolecular pump.

The **electronics service switch** is a circuit breaker that allows service of the non-vacuum system components of the mass spectrometer with the vacuum system still in operation (see Figure 2-7). In the Service Mode position the

switch removes power to all components of the mass spectrometer other than the vacuum system. In the Operational Mode position power is supplied to all components of the mass spectrometer.

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

After the electronics service switch, power goes to the +5 V, ± 15 V, +24 V, +60 V switching power supply (PS2) and the Interlock PCB.

The **+5 V, ± 15 V, +24 V, +60 V dc switching power supply (PS2)** provides +5 V dc, ± 15 V dc for analog and digital circuits. The +60 V dc is used by the heater that heats the ion transfer tube. The +24 V dc goes to the Interlock PCB and the Source PCB.

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

The **Interlock PCB** receives 220 V ac from the Power Entry Module and +24 V dc from PS2. If the safety interlock switch on the API source is closed, then the Interlock PCB distributes 220 V ac to the APCI vaporizer heater and the +33 V, -28 V switching power supply (PS3), and +24 V dc to the 8 KV power supply.

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

The **+33 V, -28 V dc switching power supply (PS3)** provides +33 V dc and -28 V dc power for the RF circuits of the RF Voltage Amplifier. It also provides +33 V dc to the DC Rod Driver PCB and the conversion dynode / electron multiplier power supply.

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

The **DC Rod Driver PCB** produces ± 330 V dc for the ion guides and mass analyzer lenses and dc offsets and ± 1 kV for the Q1 and Q3 dc rod drivers.

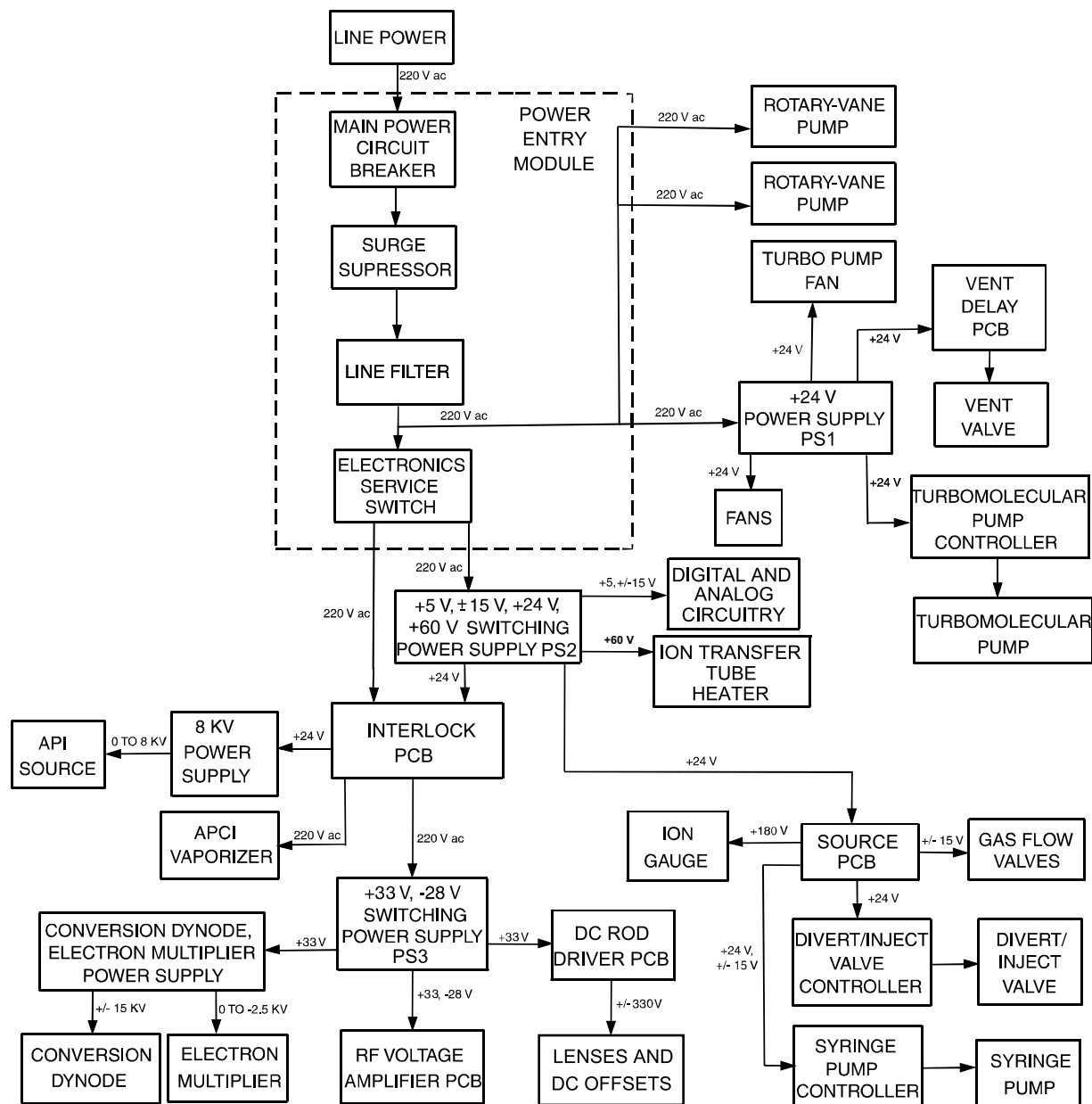


Figure 2-28. Functional block diagram of the Power Entry Module and power distribution of the mass spectrometer

System Control PCB and Embedded Computer

The “brains” of the TSQ Quantum system is the System Control PCB. The System Control PCB and embedded computer include the following:

- PowerPC processor
- Serial Peripheral Interconnect (SPI) bus
- I/O coprocessor
- Super Harvard Architecture Computer (Sharc) bus
- Scan Generator DSP
- Acquisition Processor DSP
- Interbus bridge
- 100 base-T Ethernet port

A functional block description of the System Control PCB is shown in Figure 2-29.

The System Control PCB has an embedded computer system built around a Motorola MPC 860 32-bit PowerPC processor and two Analog Devices digital signal processors (DSPs). The **PowerPC processor** handles low speed functions of the mass spectrometer such as gas control, heater regulation, pressure monitoring, and all readbacks. It sets system parameters and monitors readbacks over the serial peripheral interconnect (SPI) bus. The **SPI bus** is a 3-wire bus with data out, data in, and clock signals.

The **I/O coprocessor** resides on the same physical chip as the PowerPC processor but is a separate microprocessor. The I/O coprocessor has nonvolatile memory that contains its IP address, the IP address of the host, and the names of the files to be retrieved from the data system PC.

The **Super Harvard Architecture Computer (Sharc) bus** is a second computer subsystem on the System Control PCB. On the Sharc bus are two floating point DSPs. One is the **Scan Generator DSP**, which initiates and controls the scanning (mass filtering) of ions. The other is the **Acquisition Processor DSP**, which handles the data that is acquired by the ion detection system.

The **interbus bridge** allows the PowerPC processor to access the Sharc bus directly so it can write to memory on the two DSPs. Each DSP has on-chip memory plus shared static random access memory (SRAM). The acquisition DSP takes mass spectral data from the ion detection system and puts it in the SRAM. The PowerPC processor then reaches over the interbus bridge and fetches the data between scans.

The System Control PCB also has a high-speed **100 base-T Ethernet port** for communication with the data system PC. Mathematically intensive functions are handled by the data system PC.

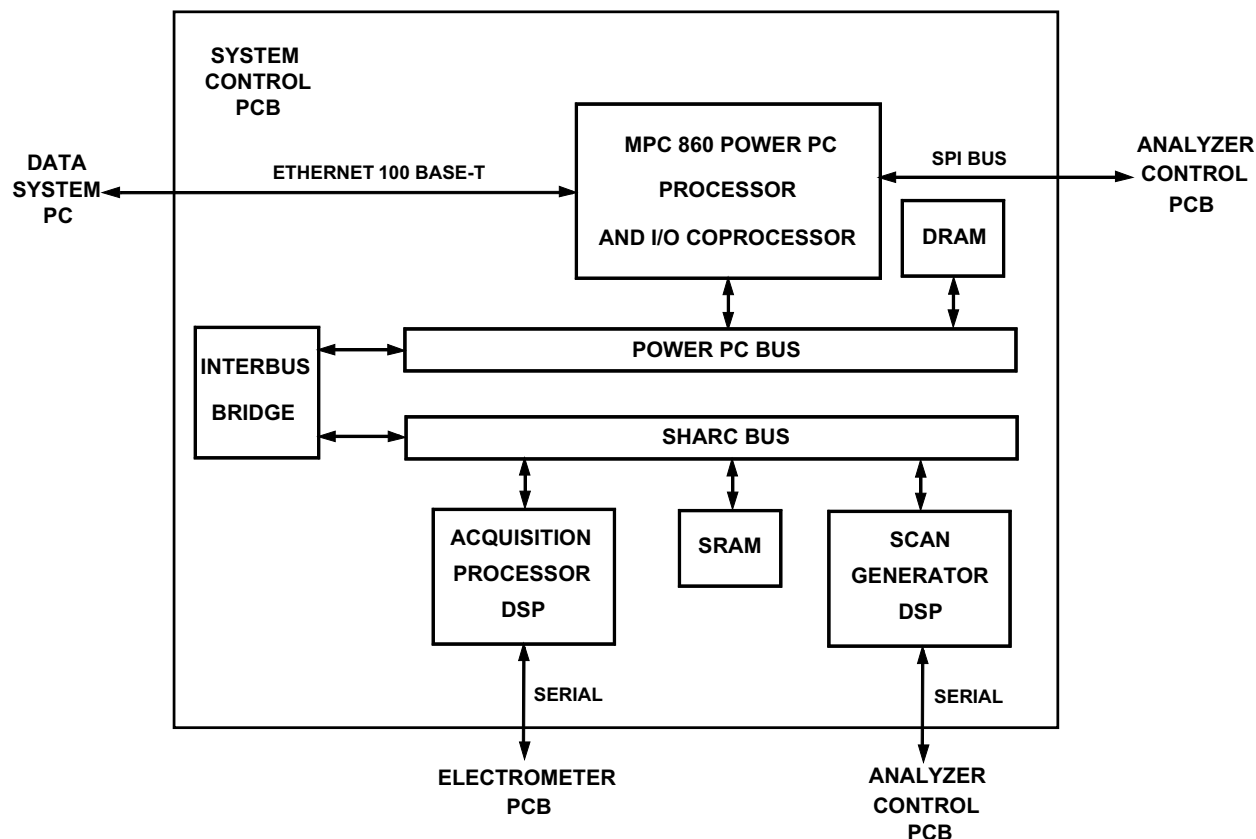


Figure 2-29. Functional block diagram of the System Control PCB

Vacuum System Electronic Assemblies

The *vacuum system electronic assemblies* control and monitor the vacuum system of the mass spectrometer. The vacuum system electronic assemblies include the following:

- System Control PCB and PowerPC processor
- Turbomolecular Pump Controller
- Vent Delay PCB
- +24 V dc switching power supply

A functional block diagram of the vacuum system electronic assemblies is shown in Figure 2-30.

The PowerPC processor on the System Control PCB monitors the pressure in the ion transfer tube-skimmer region of the vacuum manifold, as measured by the Convectron gauge, and in the analyzer region of the vacuum manifold, as measured by the ion gauge. The Convectron gauge and ion gauge signals are

sent to the PowerPC processor on the System Control PCB through analog to digital converters (ADCs) that are connected to the SPI bus. The PowerPC processor also monitors the status of the turbomolecular pump.

To prevent arcing in the analyzer region of the vacuum manifold, the System Control PCB turns off power to the mass analyzer RF voltage generation circuitry and electron multiplier and conversion dynode power supply if either one of the following conditions arise:

- The pressure in the ion transfer tube-skimmer region is above 5 Torr
- The pressure in the analyzer region is above 8×10^{-6} Torr with collision gas turned off, or 10^{-5} Torr with collision gas turned on.

The LED labeled *Vacuum* on the front panel of the TSQ Quantum instrument is illuminated green whenever the vacuum protection readbacks indicate that the vacuum is OK.

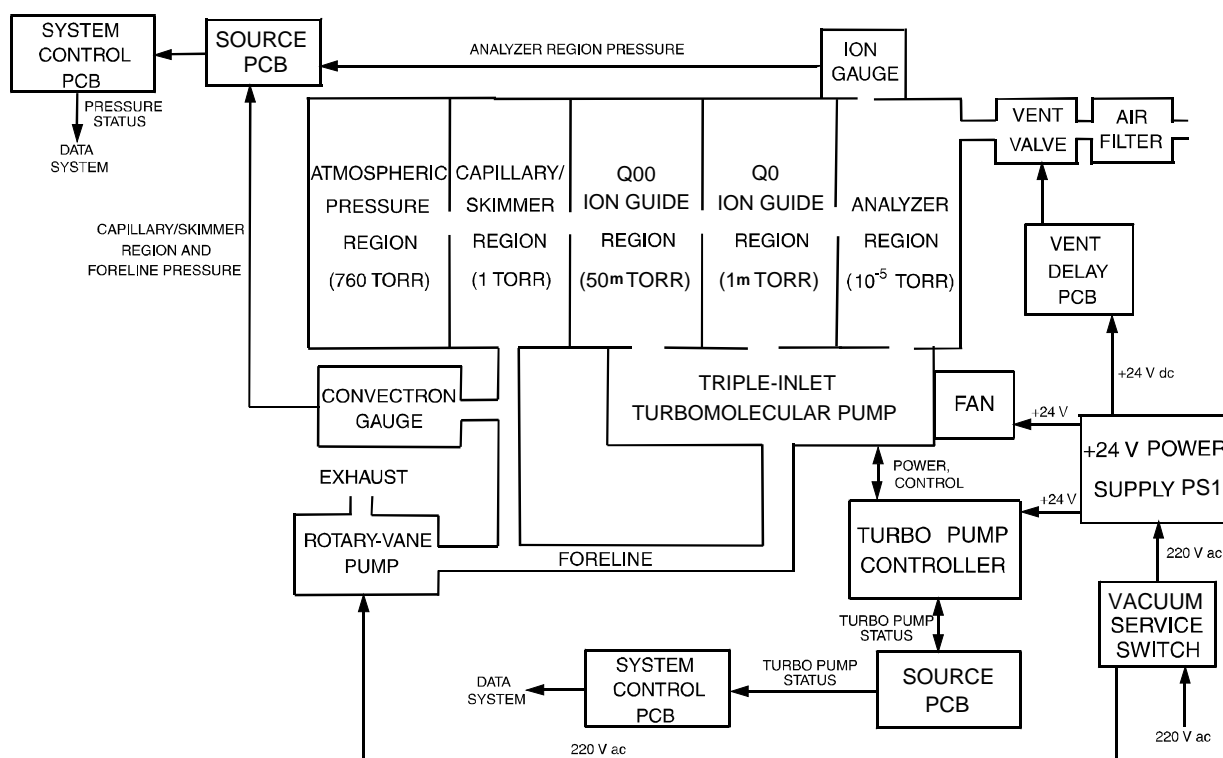


Figure 2-30. Functional block diagram of the vacuum system electronic assemblies

The **Turbomolecular Pump Controller** provides power to and control of the turbomolecular pump. The turbomolecular pump status (temperature, rotational speed, and so on) is sent from the Turbomolecular Pump Controller to the System Control PCB over a serial line. Power for the Turbomolecular Pump Controller and the turbomolecular pump is turned off and on by the main power circuit breaker and the vacuum service switch, but not by the electronics service switch.

The **Vent Delay PCB** controls the vent valve. The vent valve is closed when the solenoid is energized. The vacuum manifold is vented to filtered air 2 to 4 min after power is removed from the system.

The **+24 V power supply (PSI)** provides +24 V power to the four fans and the turbomolecular pump controller, which powers the turbomolecular pump. It also provides power to the Vent Delay PCB and vent valve during normal operating conditions. A 4-farad capacitor in the Power Entry Module provides power to the vent valve solenoid during a power failure. If external power is not restored to the instrument after 2 to 4 min, a circuit on the Vent Delay PCB times out and power to the vent valve solenoid is shut off. When power to the vent valve solenoid is shut off, the vent valve opens and the manifold is vented to filtered air. The vent valve closes after power is restored to the system.

RF Voltage Generation Electronic Assemblies

The **RF voltage generation electronic assemblies** produce the Q00, Q0, Q1, Q2, and Q3 RF voltages that enable ion transmission and mass analysis. All RF voltages are controlled by the Analyzer Control PCB and the System Control PCB.

The Q1 and Q3 RF voltage amplifier circuits are identical, and the circuits for Q00, Q0, and Q2 are similar. Thus, only the Q1 circuit will be described. The differences between the Q00, Q0, and Q2 circuits and the Q1 and Q3 circuits will be discussed as needed.

The RF voltage generation electronic assemblies include the following components. See Figure 2-31.

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

The **RF oscillator** on the Analyzer Control PCB provides a 1.123 MHz sine wave reference signal that it uses to produce the Q1 RF voltage.

The **RF Voltage Amplifier PCB** produces the 0 to 200 V ac Q1 RF primary voltage for the RF voltage coil. To produce the RF primary voltage, the RF Voltage Amplifier PCB takes the sine wave reference signal and amplifies it by an amount based on a 0 to 10 V dc RF modulation signal from the integrating amplifier.

The **Low Pass Filter PCB** removes second and third harmonics from the Q1 RF primary voltage.

The **RF voltage coil** amplifies the RF primary voltage to produce a secondary voltage of 0 to 10000 V ac (peak to peak) that is supplied to the rods of the Q1 hyperquad. Also, the two dc voltages (same magnitude, different polarity) that are applied to alternate rods are added to the RF voltage at the RF voltage coil. The two dc voltages are provided by the **DC Rod Driver PCB** and are proportional to the detected RF signal.

The **RF voltage detector** senses the 0 to 10000 V RF voltage signal applied to the hyperquad rods and converts this sensed signal into a 0 to -10 V dc output signal.

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

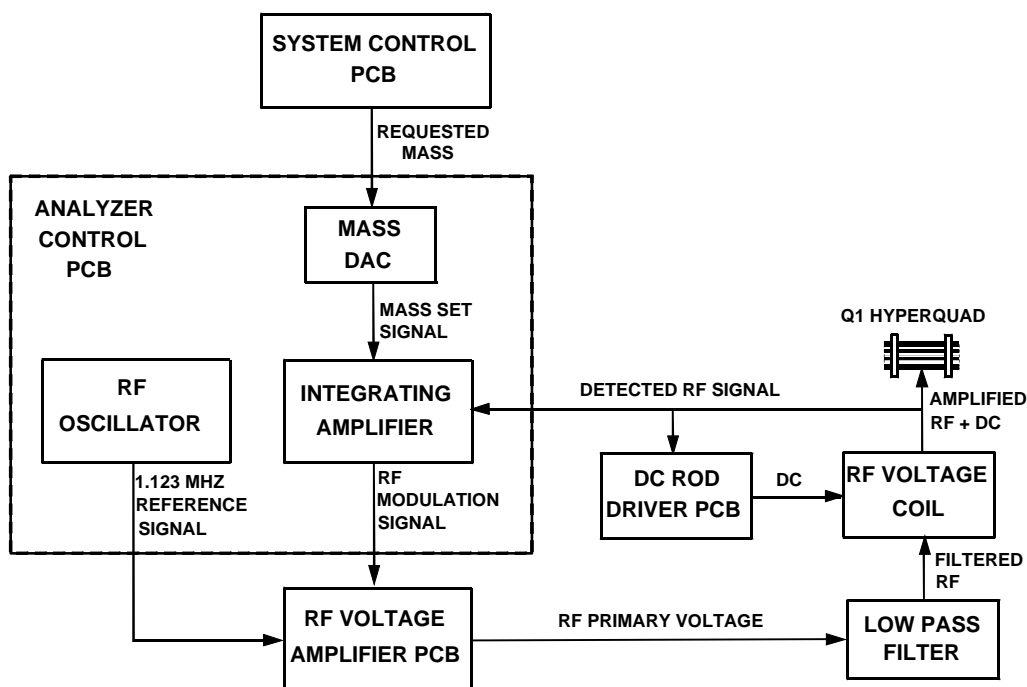


Figure 2-31. Functional block diagram of Q1 (or Q3) RF voltage generation electronic assemblies

The Q1 (and Q3) RF voltage circuit is tuned (efficiency maximized) by changing the orientation of a shorting loop inside the RF voltage coil. The shorting loop, which is rotated by a stepping motor, can either do nothing or short out a few windings of the coil, depending on its orientation. Shorting out a few windings of the coil causes the inductance to go down and the frequency to go up. The tuning circuit varies the shorting loop orientation (and thus the coil inductance) until it finds a minimum in the RF modulation signal. This occurs when the efficiency of the RF voltage circuit is at its maximum.

The circuitry for producing the Q00, Q0, and Q2 RF voltages are similar to that in Figure 2-32, except that all elements are contained on the Analyzer Control PCB. Q0 and Q00 share a doubly wound coil, and Q2 uses a different coil. The Q00, Q0, and Q2 RF voltage circuits are driven at 2.75 MHz by diodes. The Q00, Q0, and Q2 RF voltage circuits are tuned by varying the voltage applied to the diodes. Increasing the voltage causes the capacitance on the diode to go down and the frequency to go up. Q00, and Q0 are tuned together and Q2 is tuned separately.

Ion Detection System Electronic Assemblies

The *ion detection system electronic assemblies* provide high voltage to the electron multiplier and conversion dynode of the ion detection system. They also receive the electron multiplier output current signal, convert it to a voltage (by the electrometer circuit), and pass it to the embedded computer. A functional block diagram of the ion detection system electronic assemblies is shown in Figure 2-32.

The ion detection system electronic assemblies include the following:

- Electron multiplier power supply
- Conversion dynode power supply
- Electrometer PCB
- Acquisition DSP

The *electron multiplier power supply* supplies the -0.8 kV to -2.5 kV dc high voltage to the cathode of the electron multiplier. The high voltage set control signal for the electron multiplier power supply comes from the System Control PCB. This signal controls a feedback control circuit and is proportional to the final high voltage to be applied to the electron multiplier cathode.

The *conversion dynode power supply* supplies +15 kV and -15 kV dc high voltage to the conversion dynode. The polarity of the voltage applied to the conversion dynode is determined by a control signal from the System Control PCB.

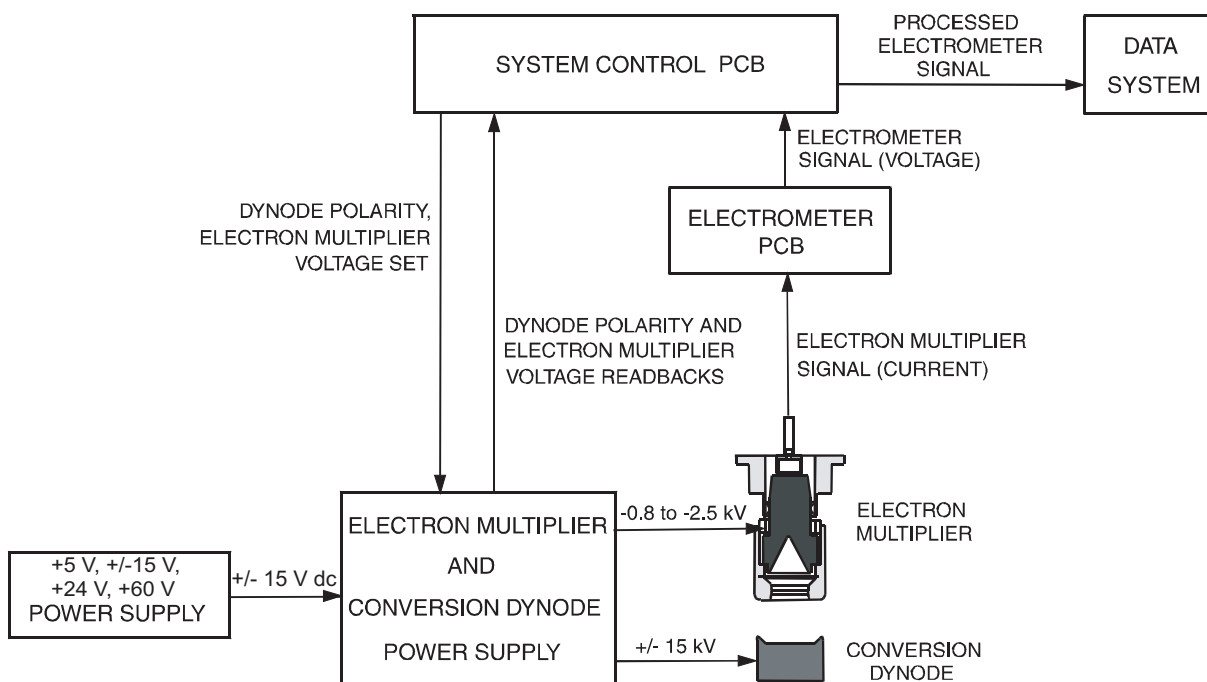


Figure 2-32. Functional block diagram of the ion detection system electronic assemblies

The *Electrometer PCB* receives the amplified ion current from the anode of the electron multiplier at a rate of 196000 samples/s, converts the current into a voltage, and then integrates the voltage over time. The integrated voltage is then passed to the Acquisition Processor DSP (on the System Control PCB) where it is processed and sent to the data system.

Analyzer Control PCB

The *Analyzer Control PCB* contains circuitry for controlling and monitoring the operation of the API source, ion guides, mass analyzer, and ion detection system. These circuits are in turn monitored by the PowerPC processor of the System Control PCB via the SPI bus.

The Analyzer Control PCB controls and monitors the RF voltages for Q00, Q0, Q1, Q2, and Q3. It also has lens voltage drivers that convert ± 330 V dc power from the DC Rod Driver PCB to dc voltages that are applied to the ion transfer tube, tube lens, lenses L0, L11, L12, L21, L22, L23, L31, L32, and L33 and quadrupoles Q00, Q0, Q1, Q2, and Q3.

2.6 Data System

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

- Computer Hardware
- Data System / Mass Spectrometer / LC Interface
- Data System / Local Area Network Interface
- Printer (optional)

Computer Hardware

The data system computer has the following major features:

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

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

Data System / Mass Spectrometer / LC Interface

The data system computer contains a 100 base-T Ethernet adapter (called the primary Ethernet adapter) that is dedicated to data system/mass spectrometer/LC communications. This primary Ethernet adapter communicates with the mass spectrometer and LC modules via a 10/100 base-T Ethernet switch (see Figure 2-27 on page 2-43). The Ethernet adapter on the mass spectrometer resides on the on the System Control PCB. A twisted pair Ethernet cable connects the primary Ethernet adapter of the data system with the Ethernet connector on the power panel of the mass spectrometer (see Figure 2-29 on page 2-48).

Data System / Local Area Network Interface

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

Printer

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

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

Chapter 3

Daily Operation

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

- Things to Do Before Operating the TSQ Quantum System
- Things to Do After Operating the TSQ Quantum System

Note. You do not need to tune and calibrate the TSQ Quantum mass spectrometer as part of your daily routine.

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

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

3.1 Things to Do Before Operating the TSQ Quantum System

The following procedures need to be performed every day before you begin your first analysis:

- Checking the Argon and Nitrogen Supplies
- Checking the ESI Fused-Silica Sample Tube for Elongation
- Checking the System Vacuum Levels
- Removing the Septum, Reinstalling the Ion Sweep Cone, and Rechecking the Vacuum Levels
- Checking the Disk Space

Checking the Argon and Nitrogen Supplies

Check the argon supply on the regulator of the gas tank. Make sure that you have sufficient gas for your analysis. If necessary, install a new tank of argon. Verify that the pressure of argon reaching the mass spectrometer is between 135 ± 70 kPa (20 ± 10 psig). If necessary, adjust the pressure with the tank pressure regulator.

Check the nitrogen supply on the regulator of the nitrogen gas tank or liquid nitrogen boil-off tank. Make sure that you have sufficient gas for your analysis. Typical nitrogen consumption is 2800 liters per day (100 cubic feet per day) (nitrogen on 24 h per day). If necessary, replace the tank. Verify that the pressure of nitrogen reaching the mass spectrometer is between 690 ± 140 kPa (100 ± 20 psig). If necessary, adjust the pressure with the tank pressure regulator.

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

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

Checking the ESI Fused-Silica Sample Tube for Elongation

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

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

To cut and reposition the sample tube 1 mm inside the end of the ESI needle, refer to the topic **Trimming the ESI Sample Tube** on page 5-21.

Checking the System Vacuum Levels

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

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

You can check the current values of the pressures in the ion transfer tube-skimmer region and foreline (labeled *Fore Press*) and in the analyzer region (labeled *Gauge Press*) in the Instrument Information Center (upper right corner) of the Quantum Tune Master window – Full Instrument Control workspace. To display the Tune Master window, from the Windows® Taskbar choose **Start > Programs > Xcalibur > Quantum Tune**. Choose **Workspace > Full Instrument Control** to display the Full Instrument Control workspace.

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

Table 3-1. Typical Pressure Readings

Conditions	Convectron gauge reading (foreline, ion transfer tube skimmer region)	Ion gauge reading (analyzer region)
Collision gas off, ion transfer tube orifice sealed	0.05 Torr	Less than 3×10^{-6} Torr (after pumping for at least one hour)
Collision gas off, ion transfer tube orifice open (250 °C)	1.2 to 1.8 Torr (110 V at 60 Hz) 1.5 to 2.2 Torr (220 V at 50 Hz)	Less than 5×10^{-6} Torr
Collision gas set to 2 mTorr, ion transfer tube orifice open (250 °C)	1.2 to 1.8 Torr (110 V at 60 Hz) 1.5 to 2.2 Torr (220 V at 50 Hz)	Less than 2×10^{-5} Torr

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

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

Removing the Septum, Reinstalling the Ion Sweep Cone, and Rechecking the Vacuum Levels

Open the lid to the API source and remove the septum from the entrance to the ion transfer tube. Reinstall the ion sweep cone on the spray cone. See Figure 3-1. Recheck the vacuum levels. Finally, close and secure the lid of the API source chamber.

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

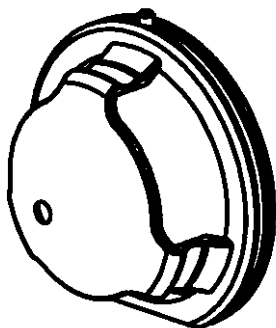


Figure 3-1. Ion sweep cone

Checking the Disk Space

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

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

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

3.2 Things to Do After Operating the TSQ Quantum System

After operating the TSQ Quantum system you need to complete the following procedures:



- Flushing the Sample Transfer Line, Sample Tube, and API Probe
- Placing the System in Standby Condition
- Flushing the Ion Sweep Cone and Ion Transfer Tube
- Capping the Ion Transfer Tube with a Septum Cap
- Purging the Oil in the Forepump
- Purging the Oil in the Forepump

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

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

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

1. Wait until data acquisition, if any, is complete.
2. Make sure that the lid to the API chamber is closed and secured.
3. From the Windows Taskbar, choose **Start > Programs > Xcalibur > Quantum Tune** to open the Quantum Tune Master window.
4. From the Quantum Tune Master window, choose **Control > On** (or click on the On/Standby button) to turn on the voltages and gas flows to the API source.
 - If you are operating in APCI mode, go to step 5.
 - If you are operating in ESI mode, go to step 6.
5. Set up the APCI source:
 - a. In the Quantum Tune Master window, choose **Workspace > Compound Optimization** to display the Optimize Compound Dependent Devices view (upper-right corner).
 - b. In the device list, click on *Vaporizer Temperature*. Then, in the text box, enter **500** and press <Enter> to set the APCI vaporizer temperature to 500 °C.
 - c. In the device list, click on *Sheath Gas Pressure*. Then, in the text box, enter **30** and press <Enter> to set the sheath gas flow rate to 30.

- d. In the device list, click on *Aux Valve Flow*. Then, in the text box, enter **5** and press **<Enter>** to set the auxiliary gas flow rate to 5.
 - e. In the device list, click on *Spray Current*. Then, in the text box, enter **0** and press **<Enter>** to set the spray current to 0.
 - f. Go to step 7.
6. Set up the ESI source:
- a. In the Quantum Tune Master window, choose **Workspace > Compound Optimization** to display the Optimize Compound Dependent Devices view (upper-right corner).
 - b. In the device list, click on *Sheath Gas Pressure*. Then, in the text box, enter **30** and press **<Enter>** to set the sheath gas flow rate to 30.
 - c. In the device list, click on *Aux Valve Flow*. Then, in the text box, enter **5** and press **<Enter>** to set the auxiliary gas flow rate to 5.
 - d. In the device list, click on *Spray Voltage*. Then, in the text box, enter **0** and press **<Enter>** to set the ESI spray voltage to 0 V.
7. Set up and start a flow of 50:50 methanol / water solution from the LC to the API source:
- a. In the Quantum Tune Master window, choose **Setup > Inlet Direct Control** (or click on the AS/LC direct control button). The Inlet Direct Control view appears.
 - b. Select the LC tab.
 - c. Set the Flow Rate to a value that is typical for your experiments.
 - d. Set the solvent proportions to 50% methanol and water.
 - e. Click on the Start button () to start the LC pump.
8. Let the solution flow through the sample transfer line, sample tube, and API probe for 15 min. After 15 min, turn off the flow of liquid from the LC to the API source, as follows. Leave the API source (including the APCI vaporizer, sheath gas, and auxiliary gas) on for an additional 5 min. Click on the Stop button () to stop the LC pump.
9. After 5 min, turn off the API source by placing the mass spectrometer in Standby: From the Quantum Tune Master window, choose **Control > Standby** (or click on the On/Standby button) to put the mass spectrometer in Standby.

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

Placing the System in Standby Condition

Use the following procedure to place the TSQ Quantum system in the standby condition:


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

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

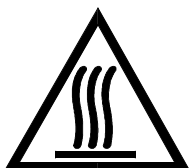
Flushing the Ion Sweep Cone and Ion Transfer Tube

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

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

1. Turn off the flow of liquid from the LC (or other sample introduction device) to the API source. To turn off the flow of liquid from the LC to the API source, do the following:
 - a. From the Windows Taskbar, choose **Start > Programs > Xcalibur > Quantum Tune** to open the Quantum Tune Master window.
 - b. In the Quantum Tune Master window, choose **Setup > Inlet Direct Control** (or click on the AS/LC direct control button). The Inlet Direct Control view appears.
 - c. Select the LC tab and click on the Stop button () to stop the LC pump.

2. From the Quantum Tune Master window, choose **Control > Standby** (or click on the On/Standby button) to put the mass spectrometer in Standby.
3. Open the lid of the API source.



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

4. Remove the ion sweep cone (Figure 3-1) from the spray cone and place it on a large Kimwipe® (or other lint-free tissue).
5. Fill a spray bottle with a 50:50 solution of HPLC-grade methanol / distilled water. Spray approximately 5 mL of the solution at the opening of the ion transfer tube. Do not touch the ion transfer tube with the tip of the spray bottle.
6. Use the spray bottle filled with the 50:50 solution of methanol / water to flush contaminants from the accessible surfaces of the ion source chamber and the spray cone.
7. Swab the ion source chamber and spray cone with a dry Kimwipe.
8. Ensure that you have removed any salt or other contaminants that may have been deposited on the ion source chamber or spray cone.
9. If you are operating in the ESI mode, wipe off the ESI nozzle with a Kimwipe soaked with the 50:50 methanol / water solution.
10. Use the spray bottle filled with the 50:50 solution of methanol / water to flush contaminants from the interior and exterior surface of the ion sweep cone. Then swab the surface of the ion sweep cone with a dry Kimwipe.

Go on to the next topic: **Capping the Ion Transfer Tube with a Septum Cap.**

Capping the Ion Transfer Tube with a Septum Cap

Place a septum over the entrance of the ion transfer tube to seal the ion transfer tube. Sealing the entrance of the ion transfer tube lessens the burden on the vacuum system and keeps contaminants out of the mass spectrometer.

Go on to the next topic: **Purging the Oil in the Forepump.**

Purging the Oil in the Forepump

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

To purge the oil in the forepump, proceed as follows:

1. Turn off the flow of sample solution from the LC to the mass spectrometer.
2. From the Quantum Tune Master window, choose **Control > Standby** (or click on the On/Standby button) to put the mass spectrometer in Standby.
3. Ensure that a septum seals the entrance to the ion transfer tube.
4. Open the gas ballast valve on the forepump by turning it to position |. Refer to the manual that came with the pump for the location of the gas ballast valve.
5. Allow the pump to run for 30 min with the gas ballast valve open.
6. After 30 min, close the gas ballast valve by turning it to position O.

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

Emptying the Solvent Waste Bottle

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

Chapter 4


Changing API Sources

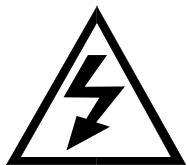
You need to change the API source (ESI or APCI) when you switch between ESI and APCI ionization modes. The ESI source consists of the ESI spray chamber housing and probe. The APCI source consists of the APCI spray chamber housing, probe, and corona discharge needle assembly. You do not need to shut down or vent the system to change the API source. The sections in this chapter are as follows:

- Removing the APCI Source
- Installing the ESI Source
- Removing the ESI Source
- Installing the APCI Source

4.1 Removing the APCI Source

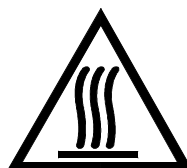
To remove the APCI source, proceed as follows.

1. Turn off the flow of liquid from the LC (or other sample introduction device) to the API source. To turn off the flow of liquid from the LC to the API source, do the following:
 - a. From the Windows Taskbar, choose **Start > Programs > Xcalibur > TSQ Tune** to open the Tune Master window.
 - b. In the Tune Master window, choose **Setup > Inlet Direct Control** (or click on the AS/LC direct control button). The Inlet Direct Control view appears.
 - c. Select the LC tab and click on the Stop button () to stop the LC pump.
2. Place the electronics service switch in the Service position. When you place the electronics service switch in the Service position, the voltages to the APCI source (including the APCI probe), ion guides, mass analyzer, and ion detection system are turned off and the flows of sheath gas and auxiliary gas into the APCI probe are stopped.



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

3. Disconnect the vaporizer heater cable from the vaporizer heater connector on the mass spectrometer. To disconnect the cable, pull back on the locking ring on the cable and turn it counterclockwise. See Figure 4-1.
4. Disconnect the sample transfer line from the APCI probe by turning the sample transfer line fitting counterclockwise until you can pull the transfer line and fitting free from the probe.
5. Remove the drain tube.
6. Open APCI source lid. Slide the lid to the left and remove it.



CAUTION. The APCI vaporizer typically operates at 400 to 600 °C and the ion transfer tube typically operates at 250 to 400 °C.

7. While you hold the APCI source housing with one hand, use a hex-head ball driver to loosen the two bolts that hold the APCI source housing to the front interface flange.
8. Pull the APCI source housing straight off.
9. Reinstall the lid on the spray chamber housing.

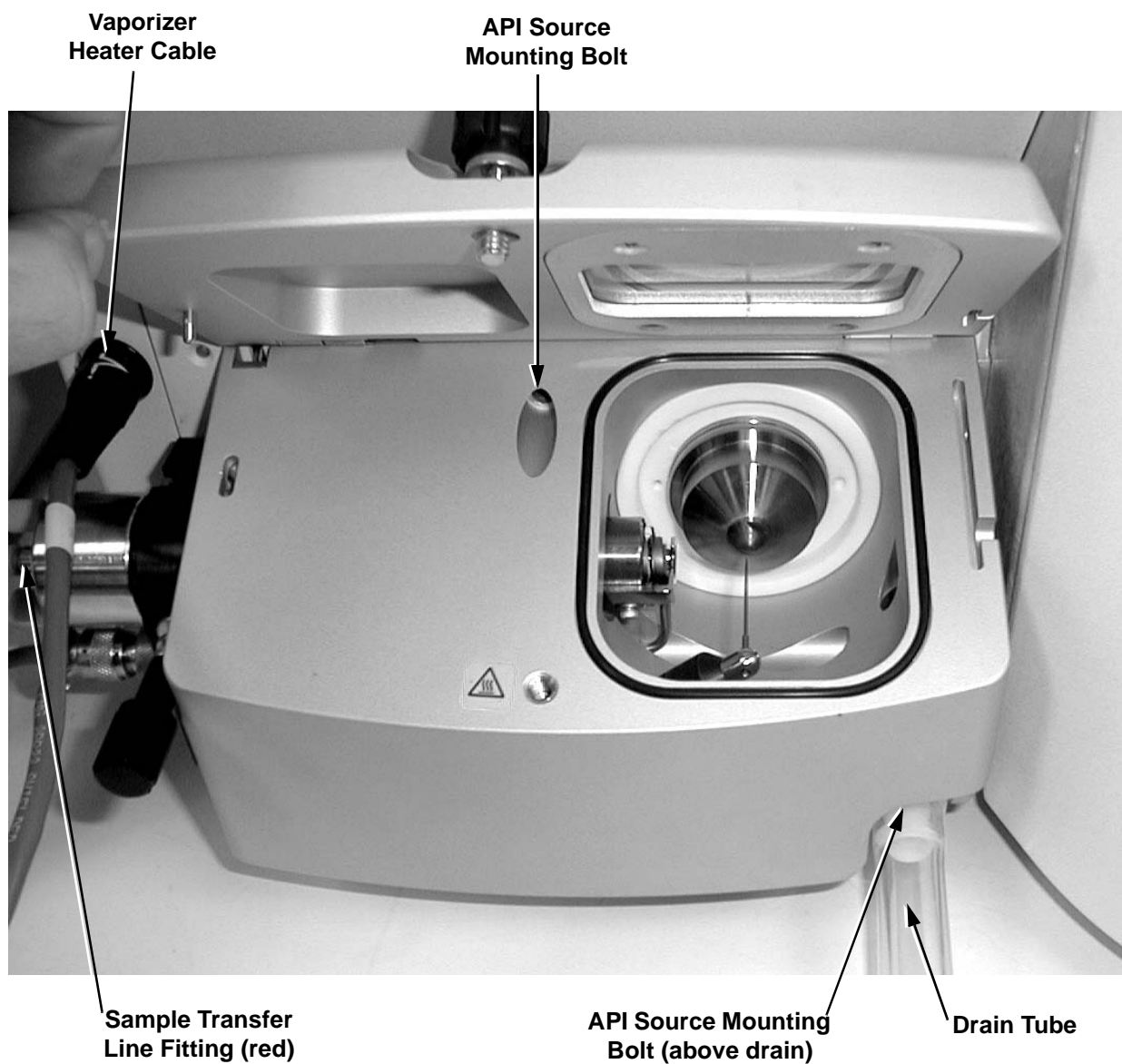
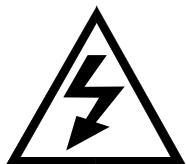


Figure 4-1. APCI source with lid open

4.2 Installing the ESI Source

To install the ESI source, remove the APCI source using the procedure described in the previous topic; then proceed as follows. Refer to Figure 4-2. for the location of the components of the ESI source.



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

Note. If your ESI source does not already contain a sample tube (fused-silica capillary), you need to follow the procedure for installing a sample tube that is outlined in the topic **Maintaining the ESI Probe** on page 5-19.

1. Place the electronics service switch in the Service position.
2. Open ESI source lid. Slide the lid to the left and remove it.
3. Align the two guide pins on the rear of the ESI source housing (see Figure 4-2) with the guide pin holes on the mass spectrometer (see Figure 4-3).
4. Push the ESI source housing onto the mass spectrometer.
5. Use a hex-head ball driver to tighten the two ESI source mounting bolts that hold the ESI source housing to the ion source interface housing.
6. Reinstall and secure the lid on the ESI source housing.
7. Connect the sample transfer line and fitting to its connector on the ESI source housing. See Figure 4-4.
8. Insert the ESI interlock plug (Figure 4-3) in the APCI vaporizer heater cable connector.
9. Attach the drain tube.
10. Place the electronics service switch in the Operational position.
11. In the Tune Master window, choose **Setup > Change Ion Source > ESI** to configure the TSQ Quantum system for ESI operation.

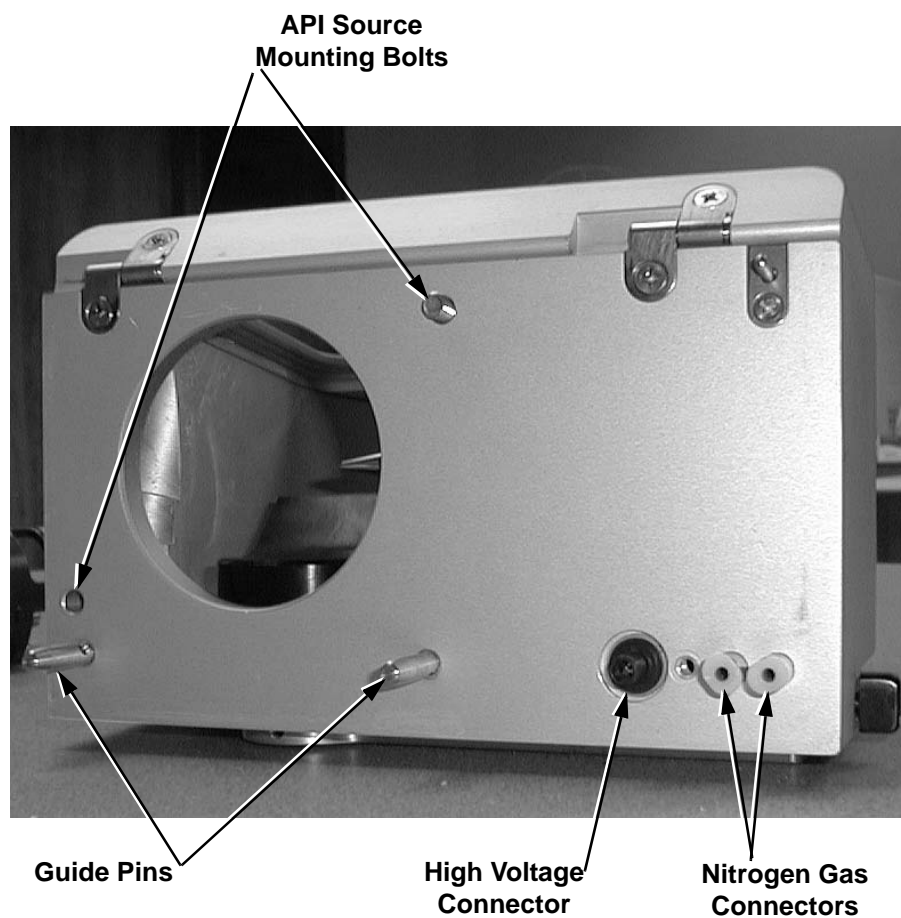


Figure 4-2. Rear view of the ESI source housing

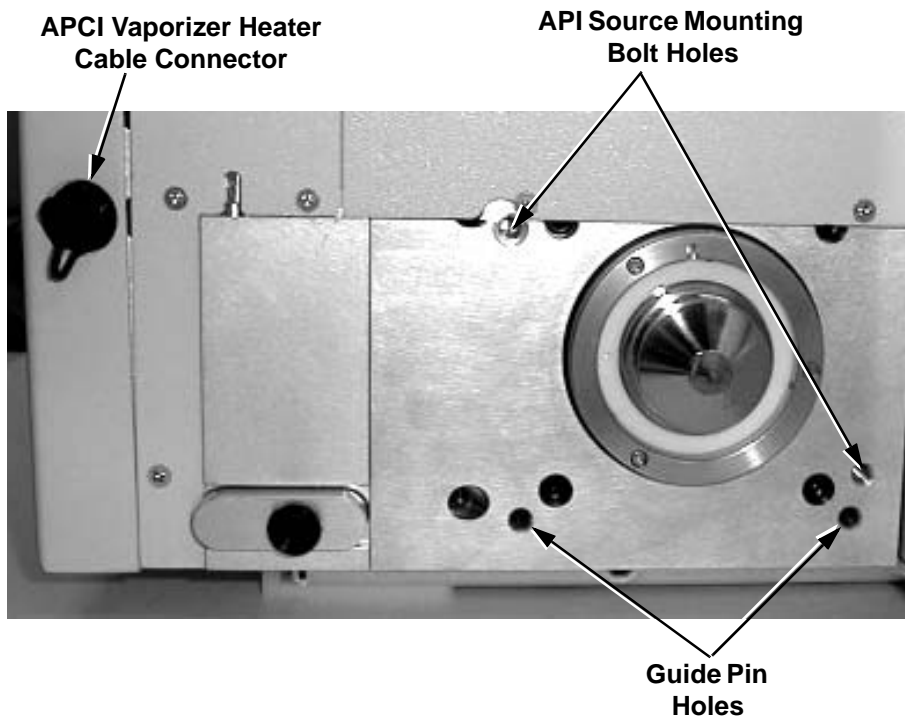


Figure 4-3. Front panel of the mass spectrometer with the API source removed

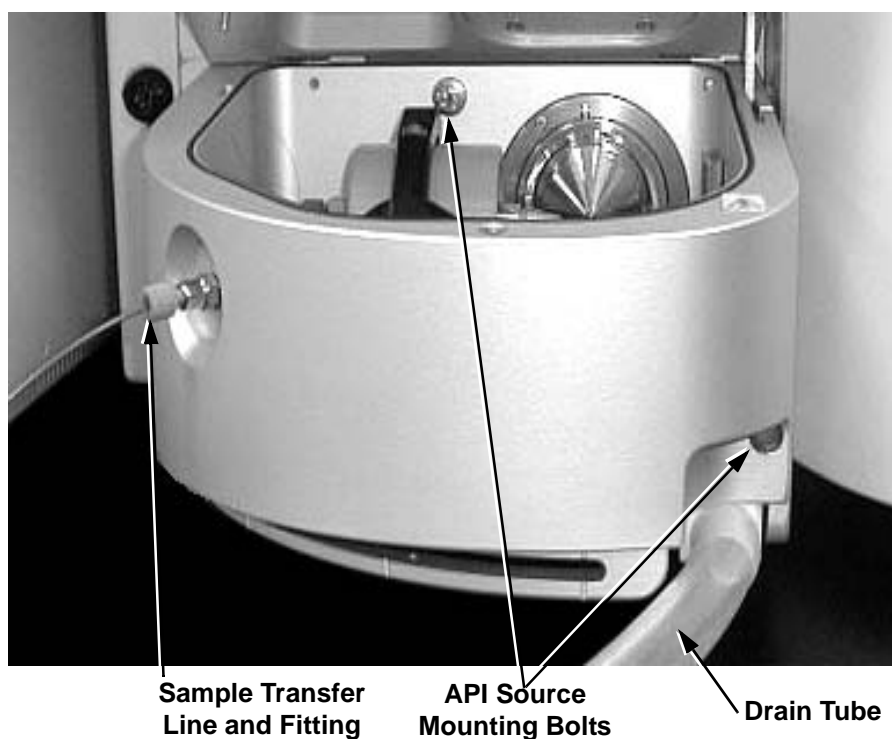



Figure 4-4. ESI source with lid open

4.3 Removing the ESI Source

This section describes how to remove the ESI source.

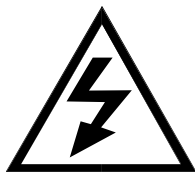
To remove the ESI source, proceed as follows.

1. Turn off the flow of liquid from the LC (or other sample introduction device) to the API source. To turn off the flow of liquid from the LC to the API source, do the following:
 - a. From the Windows Taskbar, choose **Start > Programs > Xcalibur > TSQ Tune** to open the Tune Master window.
 - b. In the Tune Master window, choose **Setup > Inlet Direct Control** (or click on the AS/LC direct control button). The Inlet Direct Control view appears.
 - c. Select the LC tab and click on the Stop button () to stop the LC pump.

Caution. Set the spray voltage to 0 V before you install the APCI source. If the spray voltage is not set to 0 V, the high voltage can cause arcing from the corona discharge needle to the API stack. Such arcing can inactivate the ion transfer tube heater. If this happens, reset the TSQ Quantum to reactivate the ion transfer tube heater.

2. Set the spray voltage of the ESI source to 0 V. To set the ESI spray voltage to 0 V, do the following:
 - a. Choose **Display > Compound Dependent Devices** (or click on the Optimize Compound Dependent Devices button). The Optimize Compound Dependent Devices view opens in the top right corner of the workspace.
 - b. In the Device Display box, click on Spray Voltage. This changes the label of the Device spin box (at the bottom of the view) to *Spray Voltage*.
 - c. In the Device spin box, enter **0** to set the spray voltage to 0 V.
3. Place the electronics service switch in the Service position.

When you place the electronics service switch in the Service position, the voltages to the API source (including the ESI probe), ion guides, mass analyzer, and ion detection system are turned off. The flows of sheath gas and auxiliary gas into the ESI probe are stopped.



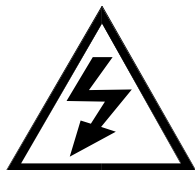
CAUTION. Make sure that the TSQ Quantum electronics service switch is in the Service position before you proceed.

4. Disconnect the sample transfer line and fitting (Figure 4-4) from its connector on the ESI source housing. (The sample transfer line is the line that comes from the LC, divert/injector valve, or syringe pump. It is not the fused silica capillary that enters the ESI probe.)
5. Remove the ESI interlock plug from the vaporizer heater cable connector on the front panel of the mass spectrometer.
6. Remove the drain tube.
7. Open ESI source lid. Slide the lid to the left and remove it.
8. While you hold the ESI source housing with one hand, use a hex-head ball driver to loosen the two API source mounting bolts that hold the ESI source housing to the front interface flange (Figure 4-4).
9. Pull the ESI source housing straight off.
10. Reinstall and secure the lid on the ESI source housing.

4.4 Installing the APCI Source

To install the APCI source, remove the ESI source using the procedure in the previous topic; then proceed as follows. Refer to Figure 4-1 on page 4-3 for the location of the components of the APCI source.

1. Place the electronics service switch in the Service position.



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

Note. If your APCI source does not already contain a sample tube (fused-silica capillary), you need to follow the procedure for installing a sample tube that is outlined in the topic **Maintaining the APCI Probe** on page 5-10.

2. Open APCI source lid. Slide the lid to the left and remove it.
3. Align the two guide pins on the rear of the APCI source housing (Figure 4-2) with the guide pin holes on the mass spectrometer (Figure 4-3).
4. Push the APCI source housing onto the mass spectrometer.
5. Use a hex-head ball driver to tighten the two API source mounting bolts that hold the APCI source housing to the ion source interface housing.
6. Reinstall and secure the lid on the APCI source housing.
7. Connect the sample transfer line and fitting to its connector on the APCI probe.
8. Connect the vaporizer heater cable to the connector on the front panel of the mass spectrometer. Make sure that the white arrow on the cable is aligned with the white line on the connector.
9. Place the electronics service switch in the Operational position.
10. In the Tune Master window, choose **Setup > Change Ion Source > APCI** to configure the TSQ Quantum system for APCI operation.

Chapter 5

Mass Spectrometer Maintenance

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

This chapter describes routine mass spectrometer maintenance procedures that must be performed to ensure optimum performance of the instrument. Most of the procedures involve cleaning. For example, procedures are provided for cleaning the ion transfer tube, the ion sweep cone, and the fan filters. Procedures are also presented for replacing the API sample tube, the ion transfer tube, and the ion source assemblies.

Routine and infrequent mass spectrometer maintenance procedures are listed in Table 5-1. For instructions on maintaining LCs or autosamplers, refer to the manual that comes with the LC or autosampler.

Table 5-1. Mass spectrometer maintenance procedures

Mass Spectrometer Component	Procedure	Frequency	Procedure Location
API source	Flush (clean) sample transfer line, sample tube, and API probe	Daily	Page 3-6
API source	Flush (clean) ion sweep cone and ion transfer tube	Daily (or more often*)	Page 3-8
Forepump	Purge (decontaminate) oil	Daily	Page 3-10
API source	Remove and clean ion transfer tube	Weekly, or if ion transfer tube bore is contaminated or obstructed	Page 5-8
API source	Replace ion transfer tube	If ion transfer tube bore is corroded	Page 5-8
Q00 ion guide	Clean tube lens and skimmer	As needed*	
Q00 ion guide	Clean Q00 quadrupole and lens L0	Every 3 to 4 months*	

Table 5-1. Mass spectrometer maintenance procedures, continued

Mass Spectrometer Component	Procedure	Frequency	Procedure Location
APCI or ESI source	Replace sample tube	If sample tube is broken or obstructed	Page 5-10 (APCI) and Page 5-19 (ESI)
ESI source	Trim sample tube	If polyimide coating on the end of the sample tube has elongated	Page 5-21
Q0 ion guide	Clean Q0 quadrupole and lenses L11 and L12**	As needed*	
Mass analyzer	Clean Q1, Q2, and Q3 quadrupoles and lenses**	As needed*	
Ion detection system	Clean ion detection system (electron multiplier and conversion dynode)**	Whenever the side cover plate of the vacuum manifold is removed	
Cooling fans	Clean fan filters	Every 4 months	Page 5-27
Forepump	Add oil	If oil level is low	Manufacturer's documentation
Forepump	Change oil	Every 3 months or if oil is cloudy or discolored	Manufacturer's documentation
Ion detection system	Replace electron multiplier assembly**	If noise in spectrum is excessive or proper electron multiplier gain can not be achieved	
Turbomolecular pump	Replace turbomolecular pump insert**	Every 20000 to 30000 hours or if bearings fail	
Electronic modules	Replace electronic module**	If electronic module fails	
PCBs	Replace PCB**	If PCB fails	
*Frequency depends on analytical conditions			
**This maintenance procedure should be performed by a Thermo Electron Field Service Engineer			

This chapter contains the following sections:

- Tools and Supplies
- Frequency of Cleaning
- API Source Maintenance
- Cleaning the Fan Filters

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

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

5.1 Tools and Supplies

The TSQ Quantum system requires very few tools for you to perform routine maintenance procedures. You can remove and disassemble many of the components by hand. The tools, equipment, and chemicals listed in Table 5-2 are needed for the maintenance of the user-maintainable components.

Table 5-2. Tools, equipment, and chemicals

Description	Part Number
Wrench, 9/16-in., socket	
Wrench, 7/16-in., open end	
Wrench, 9/16-in., open end	
Wrench, 5/16-in., open end	
Wrench, 1/2-in., open end	
Wrench, 3/8-in., open end	
Screwdrivers, set, ball point, Allen (also referred to as ball drivers)	00025-03025
Hex ball driver, 3/16-in.	00025-01700
Hex ball driver, 7/64-in.	00025-01800
Hex ball driver, 5/16-in., 9.5 in. long	00025-10015
Hex ball driver, 5/32, 7.4 in. long	00025-10020
Screwdriver, slot head, large	
Screwdriver, slot head, small	
Screwdriver, Phillips, small	
Fused-silica cutting tool	
Hypodermic tube	00106-20000
Spray bottle	
Beaker, 450 mL	
Gloves, nylon	00301-09700
Kimwipes or other lint-free industrial tissue	
Applicators (swabs), cotton-tipped	00301-02000
Detergent	
Clean, dry, compressed nitrogen gas	
Distilled water	
Methanol, HPLC grade or better	



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

5.2 Frequency of Cleaning

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

The sample tube, API probe, ion transfer tube bore, and ion sweep cone of the API source should be cleaned at the end of each operating day to remove any residual salts from buffered mobile phases or other contamination that might have accumulated during normal operation. Refer to the topics **Flushing the Sample Transfer Line, Sample Tube, and API Probe** on page 3-6 and **Flushing the Ion Sweep Cone and Ion Transfer Tube** on page 3-8.

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

- Clean the API probe, ion sweep cone, and ion transfer tube
- Clean the tube lens and skimmer

Generally, you should not open the vacuum manifold. Cleaning of the Q0, Q1, Q2, and Q3 quadrupoles is rarely (if ever) required. If you believe that cleaning of the Q0, Q1, Q2, or Q3 quadrupoles is required, you should contact Thermo Electron and schedule a visit by a Thermo Electron Field Service Engineer.

If the vacuum manifold is opened, the electron multiplier and conversion dynode should be cleaned. If the vacuum manifold is not opened, the electron multiplier and conversion dynode do not normally require cleaning, although occasionally, they might require replacement.

5.3 API Source Maintenance

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

Maintenance procedures provided below describe the following:

- Flushing the Sample Transfer Line, Sample Tube, and API Probe
- Flushing the Ion Sweep Cone and Ion Transfer Tube
- Removing and Cleaning the Ion Transfer Tube
- Maintaining the APCI Probe
- Maintaining the ESI Probe

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



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

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

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

Flushing the Ion Sweep Cone and Ion Transfer Tube


You need to clean the ion sweep cone and the ion transfer tube on a regular basis to prevent corrosion and to maintain optimum performance of your API source. A good practice is to flush the ion sweep cone and ion transfer tube at the end of each operating day after you flush the sample transfer line, sample tube, and API probe with a 50:50 methanol / water solution from the LC. To clean the ion sweep cone and the ion transfer tube follow the procedure described in the topic **Flushing the Ion Sweep Cone and Ion Transfer Tube** on page 3-8.

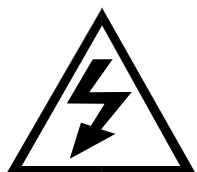
Removing and Cleaning the Ion Transfer Tube

The bore of the ion transfer tube can become blocked by buffer salts or high concentrations of sample. The ion transfer tube can be easily removed for cleaning. You do not have to vent the system to remove 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, you should suspect a blocked ion transfer tube. You can check the Convectron gauge pressure by choosing **Display > Instrument Information Center** from the Tune Master window. The pressure is listed under *Fore Press*.

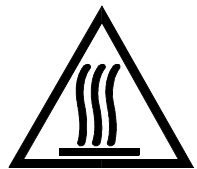
To remove and clean the ion transfer tube, do the following:

1. Turn off the flow of liquid from the LC (or other sample introduction device) to the API source. To turn off the flow of liquid from the LC to the API source, do the following:
 - a. From the Windows Taskbar, choose **Start > Programs > Xcalibur > Quantum Tune** to open the Tune Master window.
 - b. In the Tune Master window, choose **Setup > Inlet Direct Control** (or click on the AS/LC direct control button). The Inlet Direct Control view appears.
 - c. Select the LC tab and click on the Stop button () to stop the LC pump.
2. Place the electronics service switch (located on the right side of the mass spectrometer) in the Service Mode position to turn off the non-vacuum system voltages.



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

3. Remove the API source housing from the front of the mass spectrometer as described in the topic **Removing the APCI Source** on page 4-2 or **Removing the ESI Source** on page 4-7.



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

4. Remove the ion sweep cone by pulling it off the ion source interface.
5. Remove the ion transfer tube (P/N 70111-20100) by turning it counterclockwise until you can pull it free from the ion source interface.
6. Soak the ion transfer tube in a dilute solution of nitric acid to remove contaminants.
7. Sonicate the ion transfer tube in distilled water.

8. Clean the ion sweep cone by wiping the inside and outside with methanol and a Kimwipe.
9. Remove, clean with methanol, and inspect the Kalrez[®] O-ring (P/N 00107-12750) that seats in the spray cone under the entrance end of the ion transfer tube. Replace it if necessary.
10. Reseat the O-ring in the spray cone.

Caution. Use caution when reinstalling the ion transfer tube:

- Ensure that everything is properly aligned to prevent stripping the threads on the ion transfer tube.
- Be careful not to bend the ion transfer tube. Rotate the tube as you insert it.

11. Insert the ion transfer tube into the heater block. Rotate the tube as you insert it. After it is inserted, turn the tube clockwise until it is finger tight.
12. Reinstall the ion sweep cone on the ion source interface.
13. Reinstall the API source housing on the mass spectrometer as described in the topic **Installing the ESI Source** on page 4-4 or **Installing the APCI Source** on page 4-9.

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

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

Maintaining the APCI Probe

The APCI probe requires a minimum of maintenance. The APCI sample tube (150- μ m ID fused-silica tubing) is preloaded at the factory. However, if the sample tube becomes obstructed with salt precipitates or is broken, you need to replace it. Also, you may need to disassemble the APCI probe so you can clean it or to replace a part.

Figure 5-1 shows the major components of the APCI probe. You do not need to vent the system to perform maintenance on the APCI probe.

Note. You should flush the APCI probe at the end of each working day by flowing a 50:50 methanol / water solution from the LC through the APCI source. Refer to the topic **Flushing the Sample Transfer Line, Sample Tube, and API Probe** on page 3-6.

Note. Wear clean gloves when you handle APCI probe components.

The following procedures are discussed in this section:

- Removing the APCI Probe
- Disassembling the APCI Probe
- Cleaning the APCI Probe Components
- Removing the APCI Sample Tube
- Installing a New APCI Sample Tube
- Reassembling the APCI Probe
- Reinstalling the APCI Probe

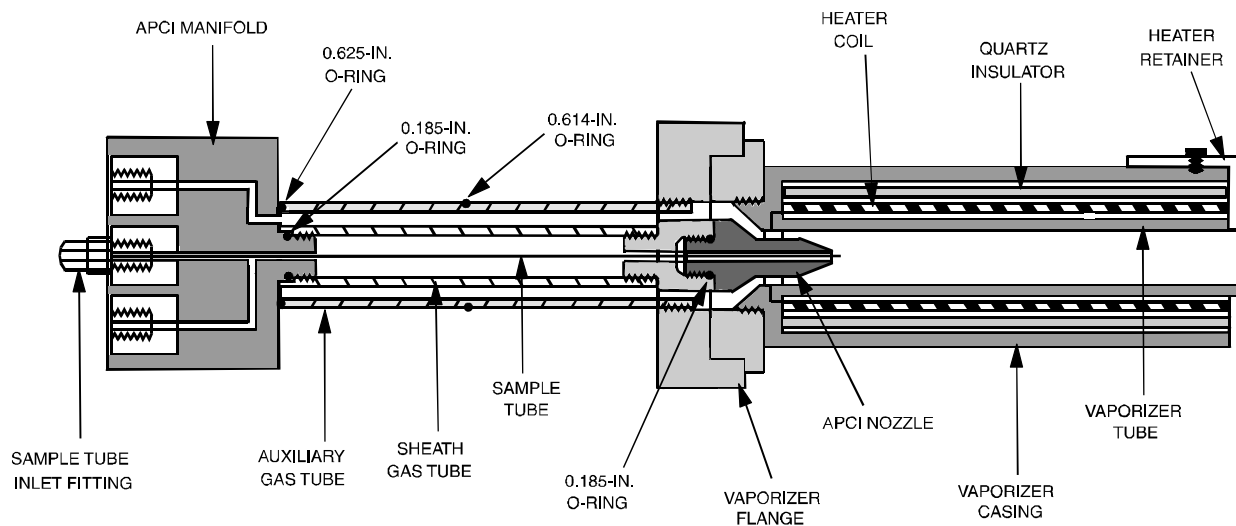
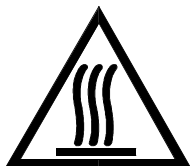


Figure 5-1. Cross sectional view of the APCI probe

Removing the APCI Probe

You do not need to remove the APCI source from the mass spectrometer in order to service the APCI probe. See Figure 5-2 for the location of the external APCI source components.



CAUTION. AVOID BURNS. The APCI vaporizer heater can reach temperatures of 600 °C. Always allow the APCI probe to cool to ambient temperatures before handling or removing the APCI probe from the APCI flange.

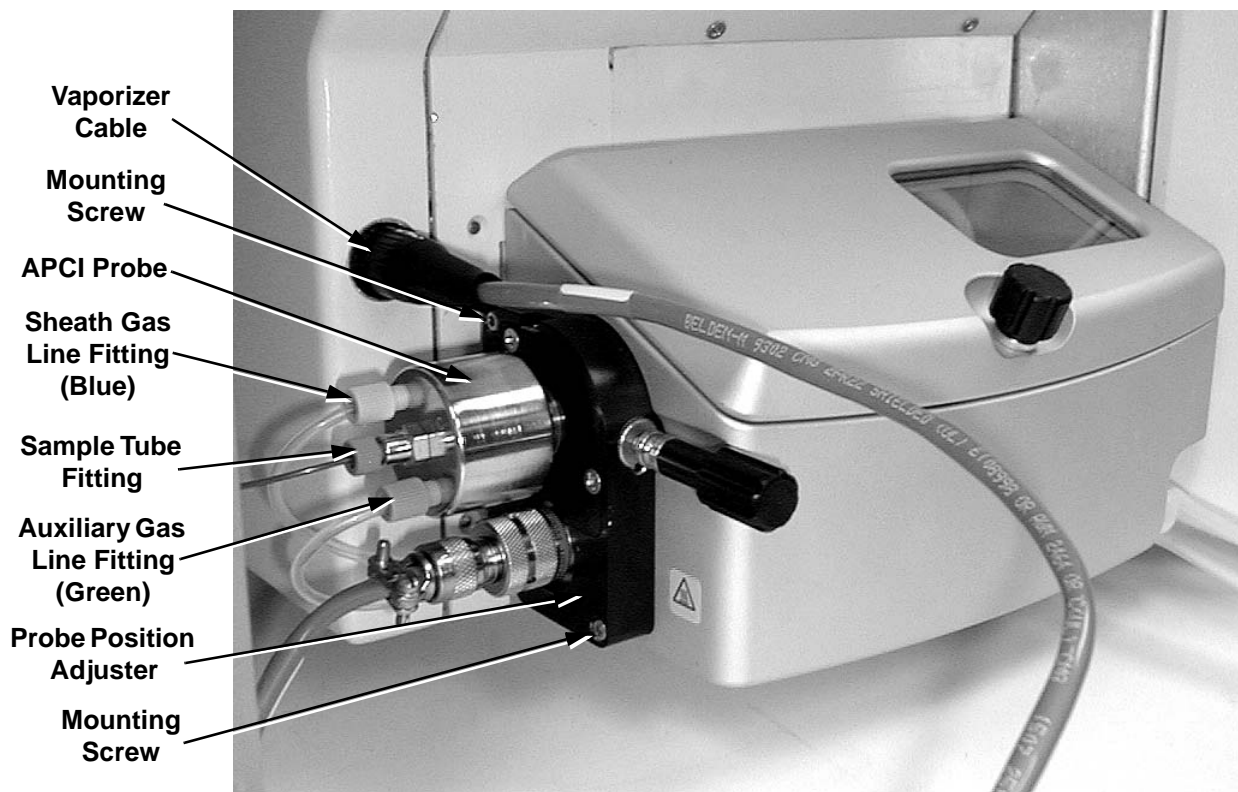
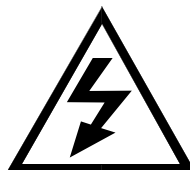


Figure 5-2. Left side of APCI source

Remove the APCI probe and probe position adjuster from the APCI source housing as follows:

1. If the APCI source is mounted on the mass spectrometer, place the electronics service switch (located on the right side of the mass spectrometer) in the Service Mode position to turn off the non-vacuum system voltages.



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

2. Disconnect the sheath gas line from the APCI probe by turning the sheath gas line fitting counterclockwise until you can pull the sheath gas line and fitting free from the probe.
3. Disconnect the auxiliary gas line from the APCI probe by turning the auxiliary gas line fitting counterclockwise until you can pull the auxiliary gas line and fitting free from the probe.
4. Disconnect the sample tube (if it is connected) from the APCI probe by turning the sample tube fitting counterclockwise until you can pull the sample tube and fitting free from the probe.
5. Disconnect the vaporizer cable from the mass spectrometer (if it is connected).
6. Loosen the two mounting screws that hold the APCI probe position adjuster to the APCI source housing.
7. Remove the APCI probe and position adjuster from the APCI source housing. Place the APCI probe and flange on a lint-free tissue and allow it to cool to ambient temperature.

Go on to the next topic: **Disassembling the APCI Probe.**

Disassembling the APCI Probe

To disassemble the APCI probe, do the following. See Figure 5-3.

Caution. Do not break the APCI sample tube. In step 1, carefully pull the APCI manifold straight back from the APCI probe to prevent the sample tube from touching the sides. If the sample tube hits the sides of the sheath gas tube, it can break.

Remove the APCI manifold and sample tube as follows:

1. Hold onto the APCI vaporizer with one hand and unscrew and remove the APCI manifold from the APCI probe. The sample tube remains with the APCI manifold.
2. Remove the vaporizer:
 - a. With an Allen wrench, remove the socket-head screw that secures the heater retainer to the vaporizer casing.
 - b. Remove the vaporizer tube, heater coil, and quartz insulator from the vaporizer.
 - c. Unscrew and remove the vaporizer casing from the vaporizer flange.

If you want to clean the APCI probe components, go on to the next topic:

Cleaning the APCI Probe Components.

If you want to replace the APCI sample tube only, go to the topic **Removing the APCI Sample Tube** on page 5-16.

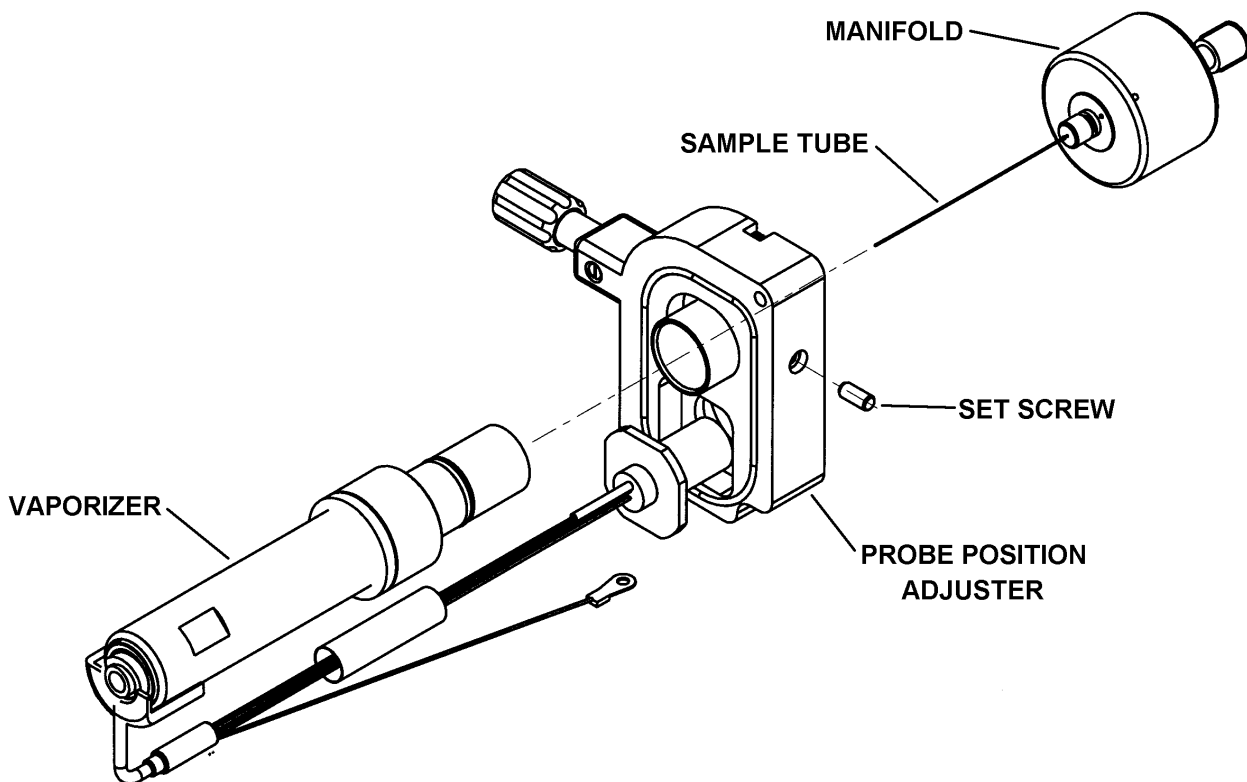


Figure 5-3. APCI probe removed from the probe position adjuster

Cleaning the APCI Probe Components

To clean the APCI probe components, proceed as follows:

1. Complete the disassembly of the APCI probe as follows. See Figure 5-1 on page 5-10 and Figure 5-4 for the location of the components.
 - a. Unscrew and remove the APCI nozzle from the vaporizer flange.
 - b. Unscrew and remove the auxiliary gas tube from the vaporizer flange.
 - c. Unscrew and remove the sheath gas tube from the vaporizer flange.
2. Remove and check the condition of the 0.185-in. ID O-ring (P/N 00107-02585) on the APCI nozzle and the 0.614-in. ID O-ring (P/N 00107-05700) and 0.625-in. ID O-ring (P/N 00107-09015) on the auxiliary gas tube. Replace the O-rings if necessary.
3. Clean the APCI components with a 50:50 solution of HPLC-grade methanol and distilled water and a lint-free swab. Dry the components with nitrogen gas and place them on a lint free tissue.

4. Reinstall the 0.614-in. and 0.625-in. O-rings on the auxiliary gas tube and the 0.185-in. O-ring on the APCI nozzle.
5. Reinstall the sheath gas tube (P/N 70005-20200) by gently screwing it by hand into the vaporizer flange.
6. Reinstall the auxiliary gas tube (P/N 70005-20199) by gently screwing it by hand into the vaporizer flange.
7. Reinstall the APCI nozzle (P/N 70005-20196) by gently screwing it by hand into the vaporizer flange.
8. Reinstall the vaporizer casing (P/N 70005-20217) by gently screwing it by hand into the vaporizer flange.

If you do not want to replace the APCI sample tube, go to the topic **Reassembling the APCI Probe** on page 5-18.

If you want to replace the APCI sample tube, go on to the next topic: **Removing the APCI Sample Tube**.

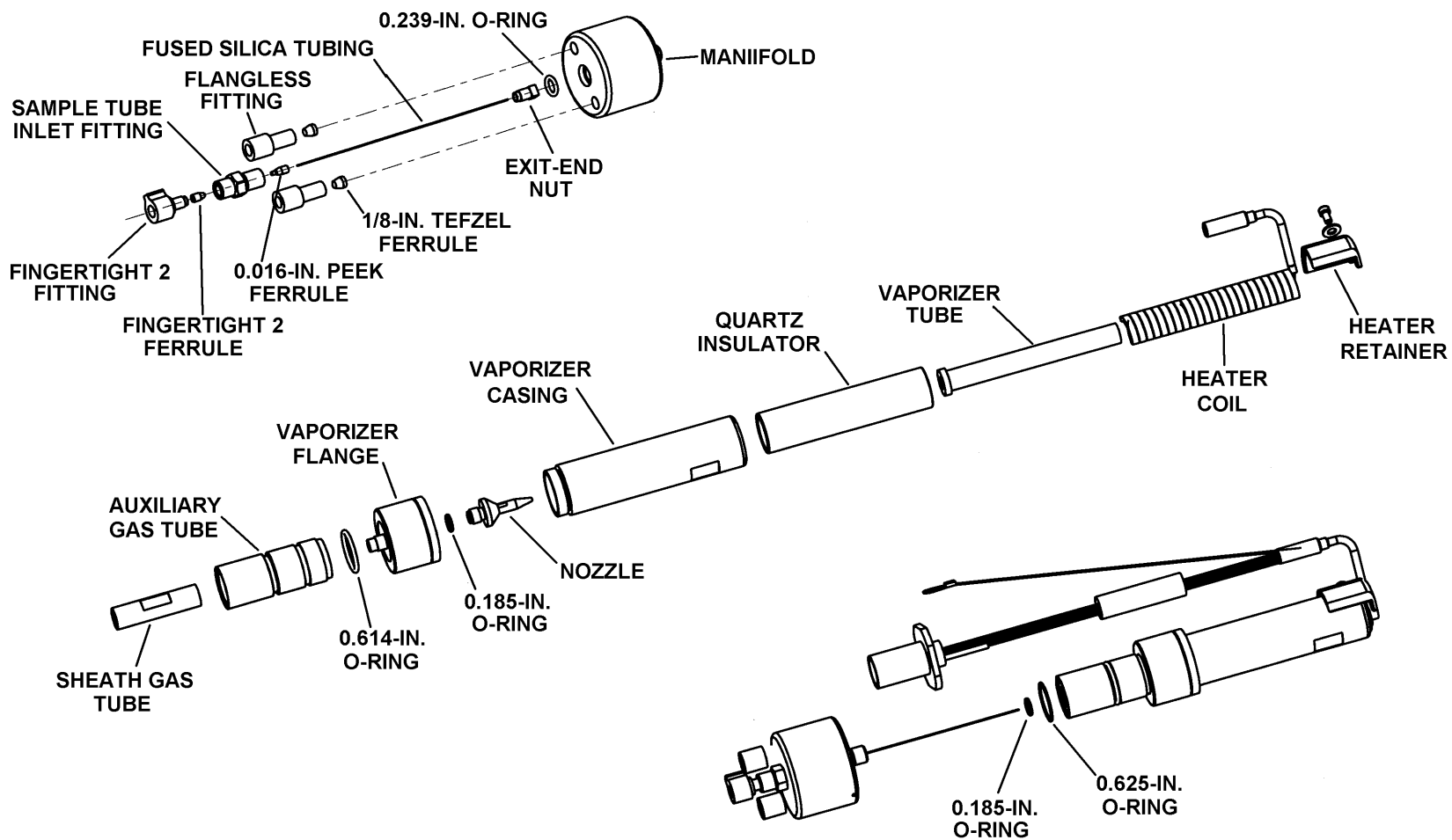


Figure 5-4. Exploded view of the APCI probe

Removing the APCI Sample Tube

To remove the APCI sample tube from the APCI manifold, do the following:

1. With a 3/8-in. open-end wrench, remove the sample tube inlet fitting (P/N 70005-20250), 0.239-in. ID O-ring (P/N 00107-04000), and sample tube from the APCI manifold. See Figure 5-5.
2. Remove the exit-end nut (P/N 70005-20220), 0.016-in. ID, PEEK ferrule (P/N 00101-18120), and sample tube from the sample tube inlet fitting.
3. Discard the old sample tube.

Go on to the next topic: **Installing a New APCI Sample Tube.**

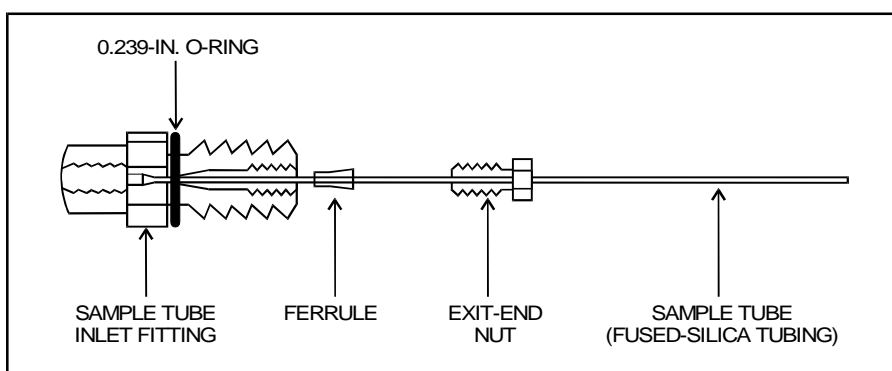


Figure 5-5. APCI sample tube connection

Installing a New APCI Sample Tube

To install a new APCI sample tube, proceed as follows:

1. Use a fused-silica cutting tool to cut a piece of 150 μ m ID, 390 μ m OD fused-silica tubing (P/N 00106-10498) to a length of approximately 15 cm (6 in.). Ensure that you squarely cut the ends of the fused-silica tubing.
2. Slide the exit-end nut (P/N 70005-20220) and ferrule (P/N 00101-18120) onto the length of the fused-silica tubing. See Figure 5-5.
3. Check the condition of the 0.239-in. ID O-ring (P/N 00107-04000) on the sample tube inlet fitting. Replace it if necessary.
4. Insert the fused-silica tubing into the sample tube inlet fitting.
5. Slide the exit-end nut and ferrule down the fused-silica tubing and into the sample tube inlet fitting.
6. Tighten the exit-end nut to secure the new sample tube (fused-silica tubing).

7. Gently slide the sample tube through the sample inlet of the APCI manifold. With a 3/8-in. open-end wrench, tighten down the sample tube inlet fitting to secure the fitting and compress the O-ring.
8. Unscrew and remove the vaporizer casing from the vaporizer flange (to expose the nozzle).
9. Gently slide the sample tube through the sheath gas tube of the APCI probe and out the APCI nozzle. Watch for the sample tube to exit the APCI nozzle. Screw the APCI manifold into the APCI probe (sheath gas tube).
10. Use a fused-silica cutting tool to cut the exit end of the sample tube so that approximately 1 mm protrudes past the tip of the APCI nozzle. See Figure 5-6.

Note. After the APCI sample tube has been cut to the proper length, you can remove the APCI manifold and accurately measure and record how far the sample tube extends past the end of the APCI manifold. The length should be about 6.5 cm (2.6 in.). In the future, sample tube replacement does not require complete disassembly of the APCI probe; just install the fused silica tubing in the APCI manifold and cut it to the proper length.

Go on to the next topic: **Reassembling the APCI Probe.**

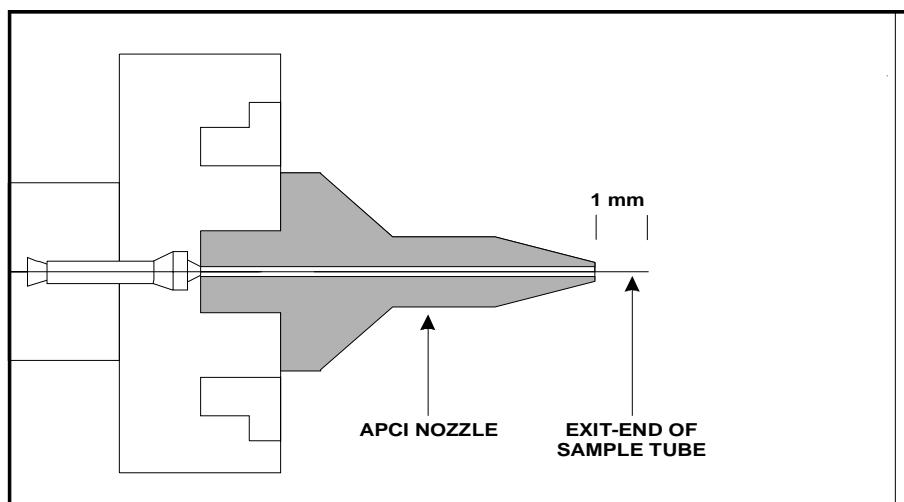


Figure 5-6. Proper position of the exit end of the APCI sample tube

Reassembling the APCI Probe

To reassemble the APCI probe, proceed as follows:

1. Unscrew and remove the APCI manifold from the APCI probe. Be careful not to damage the sample tube.
2. Gently screw the vaporizer casing back into the vaporizer flange.
3. Reinstall the heater coil and quartz insulator into the vaporizer casing.
4. Reinstall the heater retainer and secure it with the socket-head screw.
5. Reinstall the APCI probe (minus the APCI manifold) into the APCI flange.
6. Carefully slide the sample tube through the APCI flange, through the sheath gas tube, and out the APCI nozzle.
7. With one hand holding the vaporizer casing to keep the probe from turning, screw the APCI manifold onto the APCI probe.
8. Move the vaporizer wires away from the vaporizer casing.

Go on to the next topic: **Reinstalling the APCI Probe.**

Reinstalling the APCI Probe

Reinstall the APCI probe and probe position adjuster into the APCI source housing as follows. See Figure 5-2 on page 5-11.

1. Insert the APCI probe and position adjuster into the APCI source housing.
2. Insert and tighten the two mounting screws that hold the probe position adjuster to the APCI source housing.
3. Reconnect the auxiliary gas line to the APCI probe by inserting the gas line with the green fitting into the inlet labeled *A*. Tighten the auxiliary gas line fitting by turning it clockwise until it is finger tight.
4. Reconnect the sheath gas line to the APCI probe by inserting the gas line with the blue fitting into the inlet labeled *S*. Tighten the sheath gas line fitting by turning it clockwise until it is finger tight.
5. If the APCI source is mounted on the mass spectrometer, reconnect the vaporizer cable to the mass spectrometer.
6. If the APCI source is mounted on the mass spectrometer, reconnect the sample tube to the APCI probe by inserting the sample tube into the inlet labeled *LC*. Tighten the (red) sample tube fitting by turning it clockwise until it is finger tight.

Maintaining the ESI Probe

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

Note. You should flush the ESI probe at the end of each working day by flowing a 50:50 HPCL-grade methanol / distilled water solution from the LC through the ESI probe. Refer to the topic **Flushing the Sample Transfer Line, Sample Tube, and API Probe** on page 3-6.

Wear clean gloves when you handle ESI probe components.

The procedures described in this topic are:

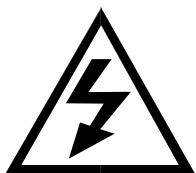
- Removing the ESI Probe
- Trimming the ESI Sample Tube
- Removing the ESI Sample Tube
- Removing the ESI Nozzle, Needle, and Needle Seal
- Cleaning the ESI Manifold
- Cleaning the ESI Nozzle
- Reassembling the ESI Probe
- Installing a New ESI Sample Tube
- Reinstalling the ESI Probe

Note. If you only want to replace the ESI sample tube, follow the procedures described in the topics **Removing the ESI Probe**, **Removing the ESI Sample Tube**, **Installing a New ESI Sample Tube**, and **Reinstalling the ESI Probe**.

Removing the ESI Probe

You do not need to remove the ESI source from the mass spectrometer to service the ESI probe.

If the ESI source is mounted on the mass spectrometer, place the electronics service switch (located on the right side of the mass spectrometer) in the Service Mode position to turn off the non-vacuum system voltages.



CAUTION. Make sure that the TSQ Quantum electronics service switch is in the Service Mode position before you proceed if the ESI source is mounted on the mass spectrometer.

To remove the ESI probe, do the following:

1. Open the lid to the ESI source. Detach the lid by pushing it to the left.
2. Disconnect the sample tube and fitting from the grounding union on the source housing by turning the fitting counterclockwise until you can pull the sample tube and fitting free from the grounding union. See Figure 5-7.
3. Loosen the screw on the probe retainer bracket. Open the probe retainer bracket by turning it to the side.
4. Unseat the ESI probe from the high-voltage and nitrogen gas connectors. Remove the ESI probe and place it on a clean surface.

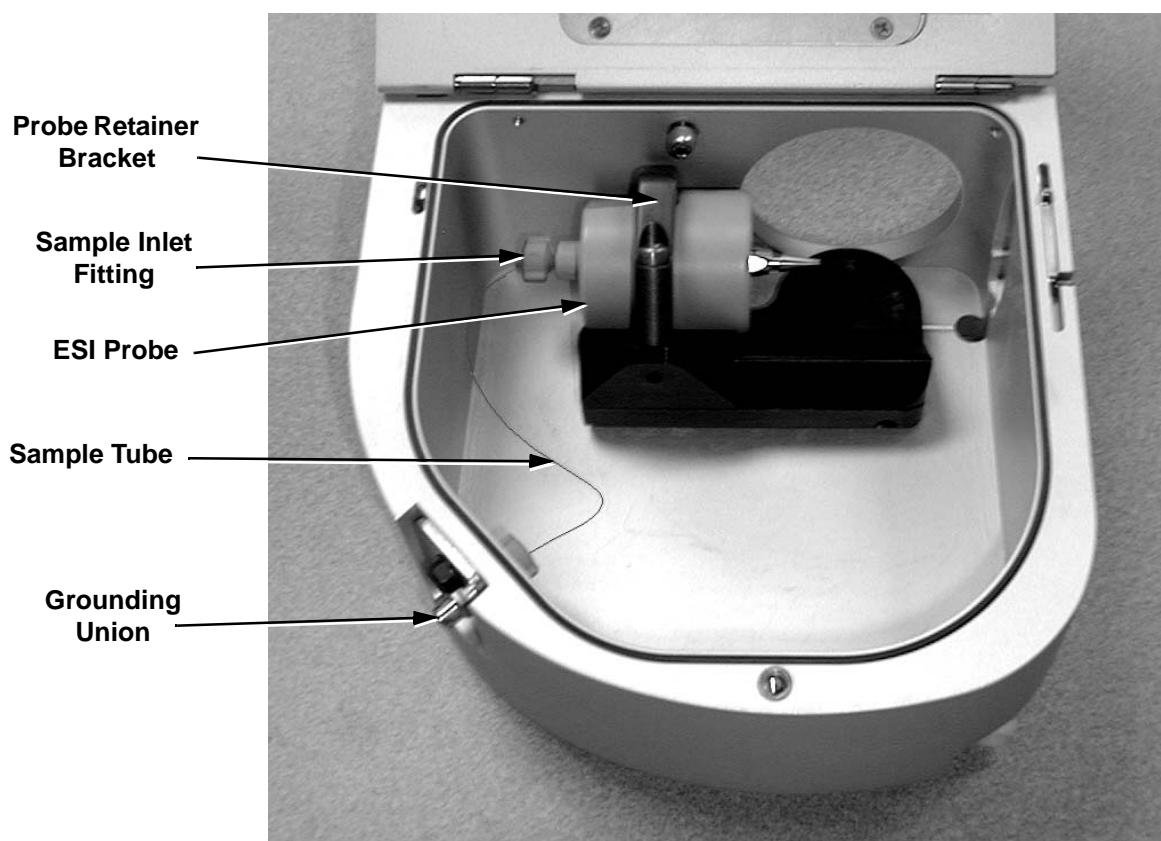


Figure 5-7. ESI probe and source housing

If you want to replace the sample tube or disassemble the ESI probe, go on to the topic **Removing the ESI Sample Tube** on page 5-21.

If you want to trim the end of the sample tube, go on to the next topic **Trimming the ESI Sample tube**.

Trimming the ESI Sample Tube

Operation of the TSQ Quantum system 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, you need to cut and reposition the end of the sample tube.

To cut and reposition the end of the sample tube 1 mm inside the end of the ESI needle, proceed as follows:

1. Remove the ESI probe from the ESI source by following the procedure described in the topic **Removing the ESI Probe** on page 5-19.
2. Loosen the sample inlet fitting.
3. Gently pull back on the sample tube to free it from the fitting.
4. Push the sample tube forward so that it extends beyond the end of the electrospray needle.
5. Use a fused-silica cutting tool to cut off a small length of sample tube. Ensure that you cut squarely the end of the sample tube.
6. Pull the sample tube backwards until the exit end of the sample tube is recessed just inside the ESI needle by approximately 1 mm.
7. Tighten the sample inlet fitting securely to hold the sample tube in place.

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

Go on to the topic **Reinstalling the ESI Probe** on page 5-26.

Removing the ESI Sample Tube

Remove the sample tube and sample inlet fitting from the ESI probe as follows:

1. Unscrew the sample inlet fitting.
2. Remove the sample tube and sample inlet fitting.

If you want to clean the interior surface of the ESI probe, go to the next topic: **Removing the ESI Nozzle, Needle, and Needle Seal**.

If you only want to replace the ESI sample tube, go to the topic **Installing a New ESI Sample Tube** on page 5-24.

Removing the ESI Nozzle, Needle, and Needle Seal

You need to remove the nozzle, needle, and needle seal to clean the ESI manifold. You need to replace the needle if it is damaged. You need to replace the needle seal if the sheath gas is leaking at the needle seal-needle interface. See Figure 5-8.

To remove the ESI nozzle, needle, and needle seal, proceed as follows:

1. Use a 5/16-in. wrench to loosen and remove the ESI nozzle from the ESI manifold.
2. Remove the ESI needle and needle seal from the ESI manifold. If necessary, after you remove the needle use the needle or another appropriate tool to push the needle seal out of the ESI manifold.
3. If necessary, replace the needle seal (P/N 00950-00952) and/or the ESI needle (P/N 00950-00990).

Go to the next topic: **Cleaning the ESI Manifold.**

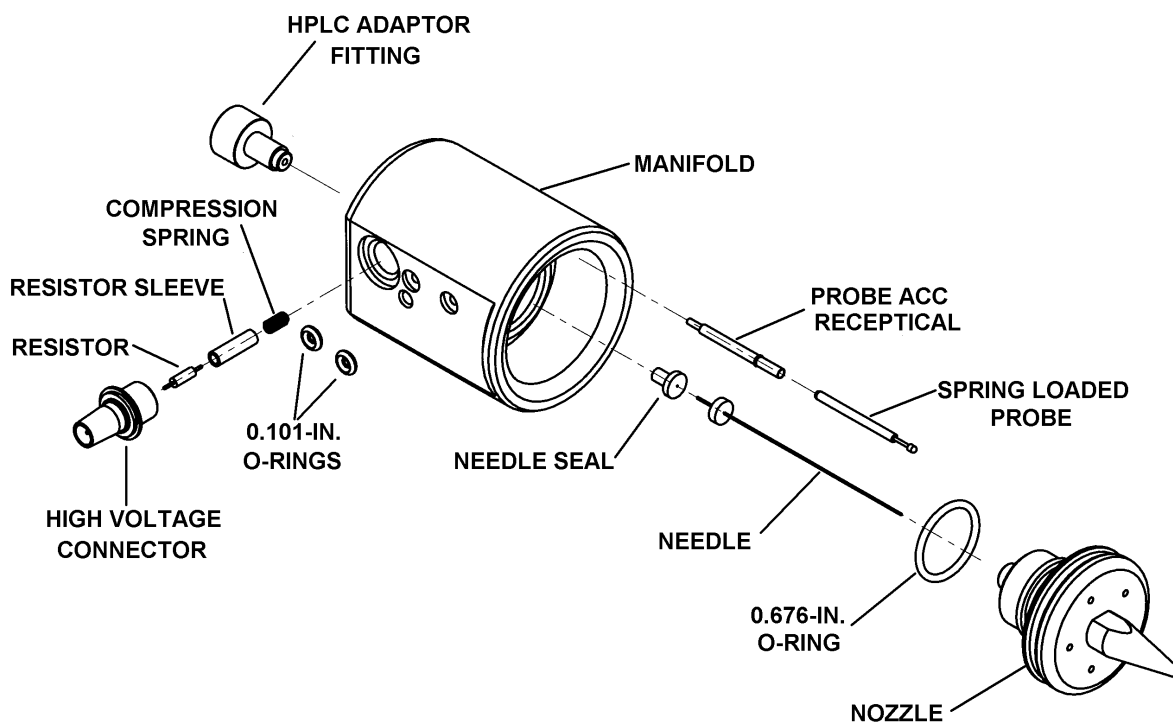


Figure 5-8. Exploded view of the ESI probe

Cleaning the ESI Manifold

To clean and dry the ESI manifold, proceed as follows:

1. If you have not already done so, remove the ESI probe following the procedure described in the topic **Removing the ESI Probe** on page 5-19.
2. If you have not already done so, use a 5/16-in. wrench to remove the ESI spray nozzle from the ESI manifold.
3. Remove the spring-loaded probe (P/N 00004-33012) and probe ACC receptacle (P/N 00004-33014) from the ESI manifold (from where it was seated behind the ESI nozzle).
4. Remove the high voltage connector (P/N 00004-95039), resistor (P/N 00015-27820), resistor sleeve (P/N 70111-20190), and compression spring (P/N 00201-11649) from the ESI manifold. Place these parts on a clean surface.
5. Rinse the ESI manifold with distilled water and then with HPLC-grade methanol. Use a Kimwipe to remove excess methanol from the ESI manifold.
6. Dry the ESI manifold with nitrogen gas.
7. Inspect all of the O-rings and replace any that are damaged.
8. Replace compression spring, resistor sleeve, resistor, and high voltage connector (that you removed in step 4) in the ESI manifold.
9. Replace probe ACC receptacle and spring loaded probe (that you removed in step 3) in the ESI manifold.

Go on to the next topic: **Cleaning the ESI Nozzle**.

Cleaning the ESI Nozzle

If necessary, clean the bore of the ESI nozzle with an appropriate solvent. This will depend on the solubility of the chemical deposits. Then rinse the nozzle with methanol and dry the nozzle with nitrogen gas.

Go on to the next topic: **Reassembling the ESI Probe**.

Reassembling the ESI Probe

To reassemble the ESI probe (that is, to reinstall the ESI sample tube, nozzle, needle, and needle seal), proceed as follows (see Figure 5-8):

1. Inspect the Teflon needle seal (P/N 00950-00952). If the needle seal is deformed, replace it.
2. Inspect the 26-gauge spray needle (P/N 00950-00990). If the spray needle is damaged, replace it.

3. Ensure that the 0.676-in. ID O-ring (P/N 00107-05710) for the sheath gas on the ESI nozzle is in good condition. In addition, ensure that the O-ring is placed into the pre-cut groove on the ESI nozzle. See Figure 5-9.
4. Reinstall the ESI nozzle, needle, and needle seal:
 - a. Insert the entrance end of the ESI needle into the needle seal.
 - b. Seat the ESI needle and needle seal in the ESI manifold.
 - c. Thread the ESI nozzle over the needle and into the ESI manifold. Slightly wet the nozzle threads with HPLC-grade methanol for lubrication.
 - d. With a 5/16-in. wrench, gently tighten the ESI nozzle until it is a little more than finger-tight. Do not overtighten the nozzle.

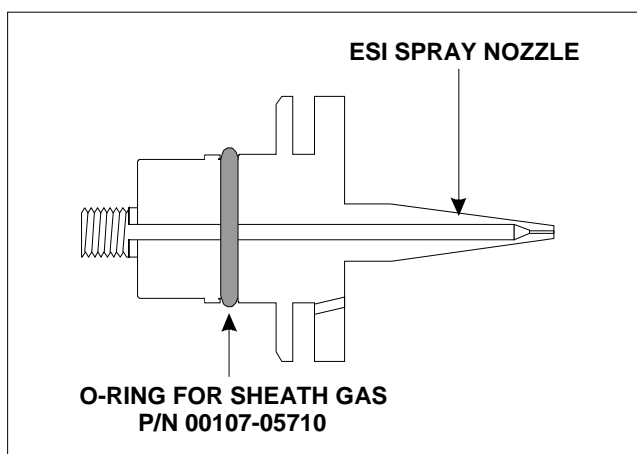


Figure 5-9. ESI spray nozzle, showing the O-ring placed in the pre-cut groove.

Go on to the next topic: **Installing a New ESI Sample Tube.**

Installing a New ESI Sample Tube

Install a new sample tube as follows:

1. Use a fused-silica cutting tool to cut a 25 cm (10-in.) to 30 cm (12-in.) piece of 0.1 mm ID \times 0.19 mm OD fused-silica tubing (sample tube) (P/N 00106-10499). Ensure that you cut squarely the ends of the fused-silica tubing.
2. Insert the sample tube through the exit end of the ESI needle and into the ESI probe.
3. Push the sample tube through the ESI probe until approximately 3.5 cm (1.5 in.) is left protruding from the exit end of the ESI needle. The remaining length of sample tube should exit the ESI probe sample inlet (labeled *Sample*).

4. Slide the 0.008-in. ID PEEK ferrule (P/N 00101-18114), narrow end first, onto the sample tube.
5. Slide the sample inlet fitting (red Fingertight fitting P/N 00101-18195) onto the sample tube and into the inlet. Tighten the fitting slightly, but not completely.
6. Pull the sample tube backwards until the exit end of the sample tube is recessed just inside the ESI needle by approximately 1 mm. See Figure 5-10.
7. Tighten the sample inlet fitting securely to hold the sample tube in place.

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

Go on to the topic: **Reinstalling the ESI Probe.**

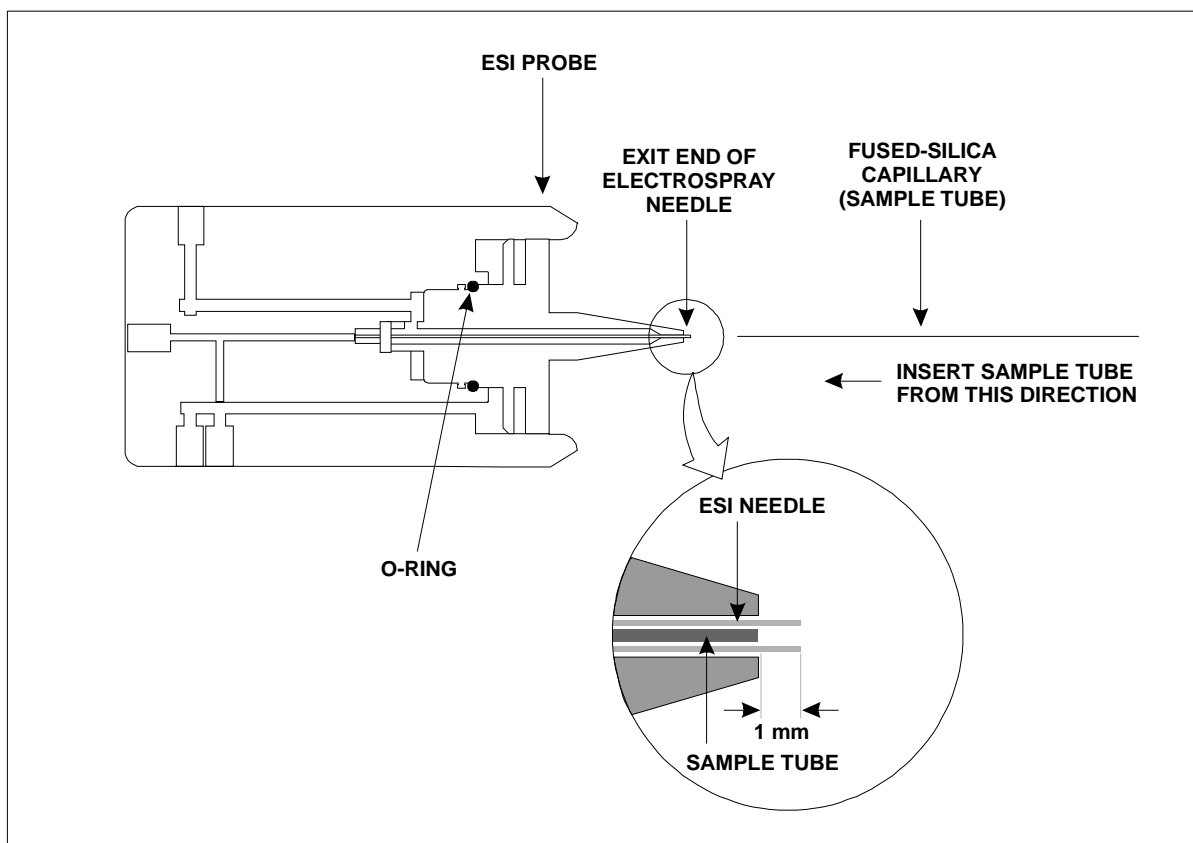


Figure 5-10. Installing the ESI fused-silica sample tube

Reinstalling the ESI Probe

To reinstall the ESI probe into the ESI source housing, do the following:

1. Ensure that the two 0.101-in. ID O-rings (Figure 5-8) are properly seated in the nitrogen inlets on the probe.
2. Seat the ESI probe onto the guide pin and high voltage and nitrogen gas connectors.
3. Turn the probe retainer bracket until it holds the ESI probe in position.
4. Slide a 1/16-in. Fingertight fitting (P/N 00101-18195) and a 0.008-in. ID, Kel-F® ferrule (P/N 00101-18114) over the free end of the sample tube.
5. Connect the free end of the sample tube to the grounding union (Figure 5-7). Make sure that the sample tube does not pass so far into the union that it is crushed when you connect the infusion transfer line.

Note. You can test the new sample tube as follows: Install the infusion transfer line onto the grounding union. Fill a 250 µL syringe with methanol and inject a small amount into the transfer line to verify that the flow is coming out the needle. The methanol should shoot straight out of the electrospray needle.

6. Reinstall the lid onto the ESI source housing.
7. In necessary, reinstall the ESI source on the TSQ Quantum instrument as described in the topic **Installing the ESI Source** on page 4-4.
8. Place the electronics service switch in the Operating Mode position.

5.4 Cleaning the Fan Filters

You need to clean the two fan filters every four months. The fan filters are located on the rear of the front cover and on the right side cover of the TSQ Quantum.

To clean the fan filters, proceed as follows:

1. Remove the fan filter from the right side cover:
 - a. Loosen and remove the four screws that hold the filter bracket to the side cover.
 - b. Remove the filter and filter bracket.
2. Remove the fan filter from the front cover:
 - a. Remove the front cover of the TSQ Quantum mass spectrometer:
 - i. Disconnect all tubing to the divert/inject valve and syringe pump.
 - ii. Depress the two (blue) spring catches that are located on either side of the front cover.
 - iii. Pull the front cover **straight off** by about 6 in (15 cm) to access the Front Panel PCB cable and grounding wire.
 - iv. Disconnect the Front Panel PCB cable from the TSQ Quantum mass spectrometer by pushing the connector retainer up and then pulling the cable free.
 - v. Pull the grounding wire free from the spade connector.
 - vi. Remove the front cover.
 - b. Loosen and remove the four screws that hold the filter bracket to the front cover.
 - c. Remove the filter and filter bracket.
3. Wash the fan filters in a solution of soap and water.
4. Rinse the fan filters with tap water.
5. Squeeze the water from the fan filters and allow them to air dry.
6. Reinstall the fan filter on the side cover:
 - a. Place the filter in the filter bracket and position the filter bracket and filter on the side cover.
 - b. Install and tighten the four screws that hold the filter bracket to the side cover.
7. Reinstall the fan filter on the front cover:
 - a. Place the filter in the filter bracket and position the filter bracket and filter on the rear of the front cover.

- b. Install and tighten the four screws that hold the filter bracket to the front cover.
- c. Reinstall the front cover of the TSQ Quantum mass spectrometer:
 - i. Position the front cover about 6 in. (15 cm) from the TSQ Quantum mass spectrometer.
 - ii. Reconnect the grounding wire to the spade connector.
 - iii. Reconnect the Front Panel PCB cable to the TSQ Quantum mass spectrometer by inserting the cable into the connector. Push the connector retainer down to secure the cable.
 - iv. Align the front cover with the two guide pins on the TSQ Quantum mass spectrometer.
 - v. Push the front cover against the TSQ Quantum mass spectrometer until the two spring catches lock.
 - vi. Reconnect all tubing to the divert/inject valve and the syringe pump.

Chapter 6

System Shutdown, Startup, and Reset

Many maintenance procedures for the TSQ Quantum system require that the mass spectrometer be shut down completely. In addition, the TSQ Quantum system can be placed in Standby if the system is not to be used for 12 h or more.

In this chapter, procedures are provided to do the following:

- Shutting Down the System in an Emergency
- Placing the System in Standby Condition
- Shutting Down the System Completely
- Starting Up the System after a Complete Shutdown
- Resetting the Mass Spectrometer
- Resetting the Data System
- Turning Off Selected Mass Spectrometer Components

6.1 Shutting Down the System in an Emergency

If you need to turn off the mass spectrometer in an emergency, place the main power circuit breaker switch, located on the power panel on the right side panel of the mass spectrometer (see Figure 6-1), in the Off (O) position. This turns off all power to the mass spectrometer, including the vacuum pumps. Although removing power abruptly will not harm any component within the system, this is not the recommended shutdown procedure to follow under normal conditions. Refer to **Shutting Down the System Completely** on page 6-4 for the recommended procedure.

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

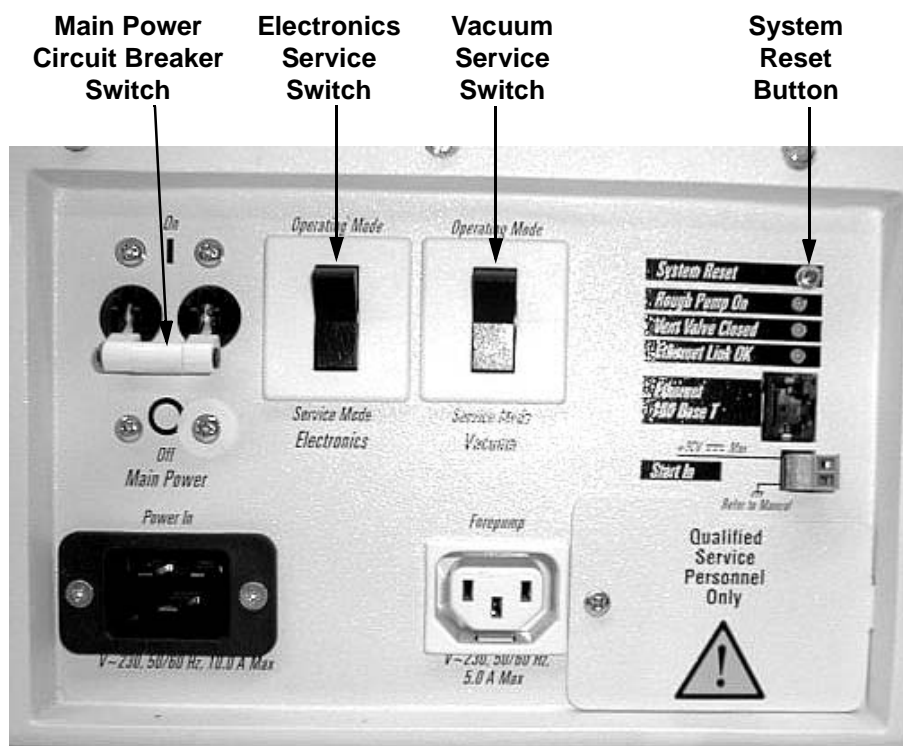



Figure 6-1. Power panel, showing the main power circuit breaker switch, electronics service switch, vacuum switch, and system reset button

6.2 Placing the System in Standby Condition

The TSQ Quantum system does not need to be shut down completely if you are not going to use it for a short period of time, such as overnight or over weekends. When you are not going to operate the system for 12 h or more, you can leave the system in a standby condition.

Use the following procedure to place the TSQ Quantum system Standby:

1. Wait until data acquisition, if any, is complete.
2. Turn off the flow of liquid from the LC (or other sample introduction device) to the API source. To turn off the flow of liquid from the LC to the API source, do the following:
 - a. From the Windows Taskbar, choose **Start > Programs > Xcalibur > Quantum Tune** to open the Tune Master window.
 - b. In the Tune Master window, choose **Setup > Inlet Direct Control** (or click on the AS/LC direct control button). The Inlet Direct Control view appears.
 - c. Select the LC tab and click on the Stop button () to stop the LC pump.
3. From the Quantum Tune Master window, choose **Control > Standby** (or click on the On/Standby button) to put the mass spectrometer in Standby.


When you choose Control > Standby, the TSQ Quantum system turns off the electron multiplier, conversion dynode, 8 kV power to the API source, and the mass analyzer and ion guide RF voltages. The TSQ Quantum system also turns off the auxiliary gas and sets the sheath gas flow to 0 units. See Table 6-1 on page 6-14 for the On/Off status of mass spectrometer components when the mass spectrometer is in the standby condition. The System LED on the front panel of the mass spectrometer is illuminated yellow when the system is in Standby.

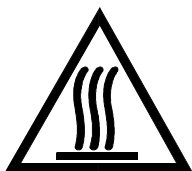
4. Flush the ion sweep cone and ion transfer tube of the API source as describe in the topic **Flushing the Ion Sweep Cone and Ion Transfer Tube** on page 3-8. Cap the ion transfer tube with the septum and close the lid on the API source.
5. Purge the forepump oil for 30 min as described in the topic **Purging the Oil in the Forepump** on page 3-10.
6. Leave the mass spectrometer power on.
7. Leave the LC power on.
8. Leave the autosampler power on.
9. Leave the data system power on.

6.3 Shutting Down the System Completely

The TSQ Quantum system does not need to be shut down completely if you are not going to use it for a short period of time, such as overnight or over weekends. (See the previous topic: **Placing the System in Standby Condition** on page 6-3.) Shut down the system completely only if it is to be unused for an extended period or if it must be shut down for a maintenance or service procedure.

Use the following procedure to shut down the TSQ Quantum system completely:

1. Turn off the flow of liquid from the LC (or other sample introduction device) to the API source. To turn off the flow of liquid from the LC to the API source, do the following:
 - a. From the Windows Taskbar, choose **Start > Programs > Xcalibur > Quantum Tune** to open the Tune Master window.
 - b. In the Tune Master window, choose **Setup > Inlet Direct Control** (or click on the AS/LC direct control button). The Inlet Direct Control view appears.
 - c. Select the LC tab and click on the Stop button () to stop the LC pump.
2. From the Quantum Tune Master window, choose **Control > Standby** (or click on the On/Standby button) to put the mass spectrometer in Standby.
3. Place the electronics service switch, located on the power panel (see Figure 6-1 on page 6-2), in the Service Mode position.
4. Place the vacuum service switch, located on the power panel (see Figure 6-1 on page 6-2), in the Service Mode position.
5. Place the main power circuit breaker switch, located on the power panel (Figure 6-1) in the Off (O) position. When you place the main power circuit breaker switch in the Off (O) position, the following occurs:
 - All power to the mass spectrometer is turned off. (All LEDs on the front panel of the mass spectrometer are off.)
 - A capacitor on the Vent Delay PCB provides power to the vent valve for 2 to 4 min (to allow the turbomolecular pump to spin down). After the capacitor discharges, power to the vent valve solenoid is shut off. When power to the vent valve solenoid is shut off, the vent valve opens and the vacuum manifold is vented to filtered air. You can hear a hissing sound as the air passes through the air filter.
 - After about 2 min, the pressure of the vacuum manifold reaches atmospheric pressure.



6. Unplug the power cord for the mass spectrometer

CAUTION. Allow heated components to cool before servicing them.

Note. If you are planning to perform routine or preventive system maintenance on the mass spectrometer only, you do not need to turn off the LC, argon and nitrogen gases, data system, or autosampler. In this case, the shutdown procedure is completed. However, if you do not plan to operate your system for an extended period of time, we recommend that you turn off the LC, data system, and autosampler as described in steps 7 through 12 below.

7. Turn off the (optional) LC. Follow the procedure described in the manual that came with the LC.
8. Turn off the argon collision gas supply at the tank.
9. Turn off the nitrogen supply at the tank.
10. Turn off the data system:
 - a. From the Windows Taskbar, choose **Start > Shut Down**. The Shut Down Windows dialog box appears.
 - b. From the list box, select *Shut Down*, and then click on **OK** to start the Windows XP shutdown procedure.
 - c. When the Windows XP shutdown procedure tells you that it is safe to turn off the computer, turn off the monitor and computer by using the on/off switches.
11. Turn off the (optional) printer by using the on/off switch.
12. Turn off the (optional) autosampler by using the main power on/off switch.

6.4 Starting Up the System after a Complete Shutdown

To start up the TSQ Quantum system after it has been shut down completely, you need to complete the following procedures:

- Starting Up the LC (optional)
- Starting Up the Data System
- Starting Up the Mass Spectrometer
- Starting Up the Autosampler (optional)
- Setting Up Conditions for Operation

Starting Up the LC

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

Starting Up the Data System

Use the following procedure to start up the data system:

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

Starting Up the Mass Spectrometer

Use the following procedure to start up the mass spectrometer.

Note. The data system must be running before you start up the mass spectrometer. The mass spectrometer will not operate until software is received from the data system.

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

4. Place the main power circuit breaker switch in the On (I) position. When you place the main power circuit breaker switch in the On (I) position, power is supplied to those mass spectrometer components that are not affected by the vacuum service switch and the electronics service switch.
5. Place the vacuum service switch in the Operating Mode position. When you place the vacuum service switch in the Operating Mode position, the forepump and the turbomolecular pump are started.
6. Place the electronics service switch in the Operational position. When you place the electronics service switch in the Operational position, the following occurs:
 - The Power LED on the mass spectrometer front panel is illuminated green to indicate that power is provided to the mass spectrometer electronics. (The electron multiplier, conversion dynode, 8 kV power to the API source, and mass analyzer and ion guide RF voltages remain off.)
 - The embedded computer reboots. After several seconds the Communication LED on the front panel is illuminated yellow to indicate that the data system and the mass spectrometer have started to establish a communication link.
 - After several more seconds, the Communication LED is illuminated green to indicate that the data system and the mass spectrometer have established a communication link. Software for the operation of the mass spectrometer is then transferred from the data system to the mass spectrometer.
 - After 3 min, the System LED is illuminated yellow to indicate that the software transfer from the data system to the mass spectrometer is complete and that the instrument is in Standby.

Note. The Vacuum LED on the front panel of the mass spectrometer remains off until the turbomolecular pump reaches 80% of its operational speed of 750 Hz. At this time the ion gauge is turned on and the Vacuum LED is illuminated yellow. The Vacuum LED is illuminated green only if the pressure in the mass analyzer region of the vacuum manifold as measured by the ion gauge is below the maximum allowable pressure of 8×10^{-6} Torr (with the collision gas turned off).

7. Place a septum cap over the ion transfer tube orifice to speed pump down.

If you have an autosampler, go on to the next topic: **Starting Up the Autosampler**. If you do not have an autosampler, go to the topic: **Setting Up Conditions for Operation** on page 6-8.

Starting Up the Autosampler

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

Setting Up Conditions for Operation

You need to do the following to set up your TSQ Quantum system for operation:

1. Before you begin data acquisition with your TSQ Quantum system, you need to allow the system to pump down for at least 1 hour. Operation of the system with excessive air and water in the vacuum manifold can cause reduced sensitivity, tuning problems, and reduced lifetime of the electron multiplier.
2. Ensure that the argon pressure and nitrogen pressure are within the operational limits [argon: 20 ± 10 psig (135 ± 70 kPa), nitrogen: 100 ± 20 psig (690 ± 140 kPa)].

<p>Note. Air in the argon line must be purged or given sufficient time to be purged for normal performance of the TSQ Quantum system.</p>
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3. Look at the Instrument Information Center or Status view in the Quantum Tune Master window. Check that the pressure measured by the ion gauge is below about 5×10^{-6} Torr, and that the pressure measured by the Convectron gauge is below about 50 mTorr (with the ion transfer tube sealed with a septum cap). (Refer to Table 3-1 on page 3-4 for normal operating pressures for the TSQ Quantum system.)
4. Remove the septum cap from the orifice of the ion transfer tube.
5. Set up for ESI or APCI operation as described in **Finnigan TSQ Quantum Getting Started**.

Note. You do not need to calibrate and tune the TSQ Quantum mass spectrometer each time you restart it.

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

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

6.5 Resetting the Mass Spectrometer

If communication between the mass spectrometer and data system computer is lost, it may be necessary to reset the mass spectrometer using the Reset button on the power panel. When you press the System Reset button, an interrupt in the embedded computer is created. This causes the embedded computer to restart in a known (default) state. See Figure 6-1 on page 6-2 for the location of the System Reset button.

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

To reset the mass spectrometer, press the System Reset button located on the power panel. Make sure the Communication LED is extinguished before releasing the System Reset button. When you press the Reset button, the following occurs:

- An interrupt on the embedded computer causes the CPU to reboot. All LEDs on the front panel of the mass spectrometer are off except the Power LED.
- After several seconds, the Communication LED is illuminated 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 is illuminated green to indicate that the data system and the mass spectrometer have established a communication link. Software for the operation of the mass spectrometer is then transferred from the data system to the mass spectrometer.
- After 3 min the software transfer is complete. The System LED is illuminated either green to indicate that the instrument is functional and the high voltages are on, or yellow to indicate that the instrument is functional, and it is in Standby.

6.6 Resetting the Data System

You can reset the data system by doing either of the following:

- Resetting the Data System by Using the Windows Shutdown and Restart Procedure
- Resetting the Data System by Turning the Personal Computer Off Then On

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

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

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

1. From the Windows Taskbar, choose **Start > Shut Down**. The Shut Down Windows dialog box appears.
2. Select *Restart* from the list box, and then click on **OK** to start the Windows XP shutdown and restart procedure.
3. Observe the Windows XP shutdown and restart procedure on the monitor. Press <Ctrl>+<Alt>+ when you are prompted to do so. Then, click on **OK** or enter your password (if you have one) in the Logon Information dialog box to complete the shutdown and restart procedure.

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

Resetting the Data System by Turning the Personal Computer Off Then On

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

1. Press the power button on the personal computer to turn the personal computer off.
2. After several seconds, press the power button on the personal computer to turn the personal computer on.
3. Observe the Windows XP startup procedure on the monitor and press **<Ctrl>+<Alt>+** when you are prompted to do so. Then, click on **OK** or enter your password (if you have one) in the Logon Information dialog box to complete the shutdown and restart procedure.
4. When the shutdown and restart procedure has completed, from the Windows Taskbar, choose **Start > Programs > Xcalibur > Quantum Tune** to display the Quantum Tune Master window.

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

6.7 Turning Off Selected Mass Spectrometer Components

There are six ways that you can turn off some or all of the mass spectrometer components:

- Turn off individual mass spectrometer components from the Quantum Tune Master window. Turning off individual mass spectrometer components might be necessary when you are troubleshooting or when you are running certain diagnostic procedures.
- Place the mass spectrometer in Standby. Standby is the normal condition to leave the mass spectrometer in when it is not in use. Choose **Control > Standby** (or toggle the On/Standby button) from the Quantum Tune Master window to place the mass spectrometer in Standby.
- Place the mass spectrometer in the Off condition. The Off condition is similar to Standby, except all high voltage components of the mass spectrometer are turned off. Choose **Control > Off** from the Quantum Tune Master window to place the mass spectrometer in the Off condition.
- Place the electronics service switch in the Service Mode position. The electronics service switch turns off all components in the mass spectrometer other than the +24 V power supply, forepump, turbomolecular pump, Vent Delay PCB, and fans.
- Place the vacuum service switch in the Service Mode position. Placing the vacuum service switch in the Service Mode position turns off power to the +24 V power supply, forepump, turbomolecular pump, Vent Delay PCB, and fans.
- Place the main power circuit breaker switch in the Off (O) position. Placing the main power circuit breaker switch in the Off (O) position removes all power to the mass spectrometer, including the vacuum system.

The on/off status of mass spectrometer components, voltages, and gas flows is summarized in Table 6-1.

Table 6-1. On/Off Status of components, voltages, and gas flows





Mass Spectrometer Component	Standby 	Off 	Electronics service switch in Service Mode position	Main power circuit breaker switch in Off (O) position
Electron multiplier	Off	Off	Off	Off
Conversion dynode	Off	Off	Off	Off
Mass analyzer RF voltage	Off	Off	Off	Off
Mass analyzer dc offset voltage	On	Off	Off	Off
Q00 and Q0 ion guide RF voltage	Off	Off	Off	Off
Q00 and Q0 ion guide dc offset voltage	On	Off	Off	Off
Tube lens	On	Off	Off	Off
Heated ion transfer tube heater	On	On	Off	Off
Heated ion transfer tube dc offset	On	Off	Off	Off
Corona discharge needle	Off	Off	Off	Off
APCI vaporizer	Off	Off	Off	Off
ESI needle	Off	Off	Off	Off
Sheath gas	Off	Off	Off	Off
Auxiliary gas	Off	Off	Off	Off
Argon collision gas	Off	Off	Off	Off
Vent valve	Closed	Closed	Closed	Open (after 2 to 4 min)
Turbomolecular pump	On	On	On	Off
Forepump	On	On	On	Off
Vent Delay PCB	On	On	On	Off
Embedded computer	On	On	Off	Off
Turbomolecular Pump Controller	On	On	On	Off
Power supply, electron multiplier and conversion dynode	Off	Off	Off	Off
Power supply, 8 kV	Off	Off	Off	Off
PS1 power supply, +24 V	On	On	On	Off

Table 6-1. On/Off Status of components, voltages, and gas flows, continued

Mass Spectrometer Component	Standby 	Off 	Electronics service switch in Service Mode position	Main power circuit breaker switch in Off (O) position
PS2 power supply, +5, ± 15 , ± 24 V dc	On	Off	Off	Off
PS3 power supply, +36, -28 V dc	On	Off	Off	Off
Fan, turbomolecular pump	On	On	On	Off
Fan, above manifold	On	On	Off	Off
Fan, center wall	On	On	On	Off
Convectron gauge, foreline	On	On	Off	Off
Convectron gauge, collision cell	On	On	Off	Off
Ion gauge	On	On	Off	Off

Chapter 7

Diagnostics and PCB and Assembly Replacement

Many of the TSQ Quantum mass spectrometer components can be tested by the TSQ Quantum diagnostics. If there is a problem with the instrument electronics, the diagnostics can often locate the problem. The problem can then be corrected by replacing a faulty PCB or assembly. After the PCB or assembly is replaced, the diagnostic tests are rerun to verify the instrument is functioning properly.

This chapter contains the following sections:

- Running the TSQ Quantum Diagnostics
- Replacing a Fuse
- Replacing PCBs and Power Supplies

Note. You can password protect several of the workspaces in the TSQ Quantum Tune Master window. The workspaces that you can protect are as follows: System Tune and Calibration, Full Instrument Control, and Diagnostics.

There are three levels of protection possible, as follows: none, automatic, and custom password. No protection means that all operators can access all workspaces. Automatic protection means that Tune Master uses the default password to protect the three protectable workspaces. The default password is *lctsq*. Custom password protection means that your Laboratory Administrator or Manager can select a password to protect the three workspaces.

If your TSQ Quantum has been password protected, you need to obtain the password before you can enter any of the three protected workspaces, including the Diagnostics workspace. If you have forgotten your password, you need to reinstall the TSQ Quantum software to reset the instrument for no password.

7.1 Running the TSQ Quantum Diagnostics

The TSQ Quantum diagnostics are used to test the major electronic circuits within the instrument and indicate whether the circuits pass or fail the tests. If there is a problem with the instrument electronics, the TSQ Quantum diagnostics can often locate the problem.

The TSQ Quantum diagnostics do not diagnose problems that are not electrical in nature. For example, they do not diagnose poor sensitivity due to misaligned or dirty components or to improper tuning. Therefore, it is important that the person running the diagnostics be familiar with the system operation and basic hardware theory as well as the details of the diagnostics.

Typically, only a Thermo Electron Field Service Engineer should run diagnostic tests because certain tests can overwrite system parameters. However, before calling a Thermo Electron Field Service Engineer to run diagnostic tests, you should consider the following:

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

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

If the answer is yes to one of the last two items above, the problem is probably mechanical, not electrical. Reverify that alignment, configurations, and cable connections are correct before you call a Thermo Electron Field Service Engineer.

Keep careful notes documenting the nature of the problem and the steps you take to correct the problem. If you are not successful in correcting the problem, you can e-mail this information to the Field Service Engineer so that a preliminary evaluation of the problem can be made before he or she arrives at your site.

7.2 Replacing a Fuse

Fuses protect the various circuits by opening the circuits whenever overcurrent occurs. On the TSQ Quantum mass spectrometer, a failed fuse indicates a failed board or electronic module that needs to be replaced by a Thermo Electron Field Service Engineer.

7.3 Replacing PCBs and Power Supplies

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

Chapter 8

Replaceable Parts

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

Note. Some parts are also available as exchange parts. An exchange part is a refurbished part that can be purchased at a discounted price. Exchange parts are specified by placing *EX* in front of the part number. For example, EX70111-60195.

This chapter contains part numbers for the following:

- Mass Spectrometer
- Data System Hardware
- Manuals
- Accessory Kit
- Metal Needle Kits
- Fittings, Ferrules, and Sample Loops

8.1 Mass Spectrometer

Replaceable parts are available to support the following:

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

However, many replaceable parts are in assemblies that should be repaired or replaced only by a Thermo Electron Field Service Engineer. Such replaceable parts are not listed in this chapter or elsewhere in this manual.

ESI Source

Housing, ESI Assembly	OPTON-20001
Probe, ESI	70111-60036
Probe, spring loaded, 6 A, SPA-3D	00004-33012
Probe ACC, receptacle, SPR-3W	00004-33014
CNTCT, battery probe, spring, 5 A, 0.512, Au	00004-95039
Resistor, FXD, CC 1/4W, 22 M, 5%	00015-27820
Fitting, HPLC adaptor, 10-32 × 1/4 in., Kel-F	00101-18080
O-ring, 0.101ID × 0.07 in., Viton (2 each)	00107-02456
O-ring, 0.676ID × 1/16 in., Viton	00107-05710
Spring, compression, 0.31 in, 0.12 in. OD, stainless steel	00201-11649
Seal, standard needle 5000 series	00950-00952
Needle, D point, 26 gauge, 2 in, 0.24 in. D washer	00950-00990
Nozzle, ESI	70111-20125
Body, probe, ESI	70111-20126
Sleeve, resistor contact	70111-20190

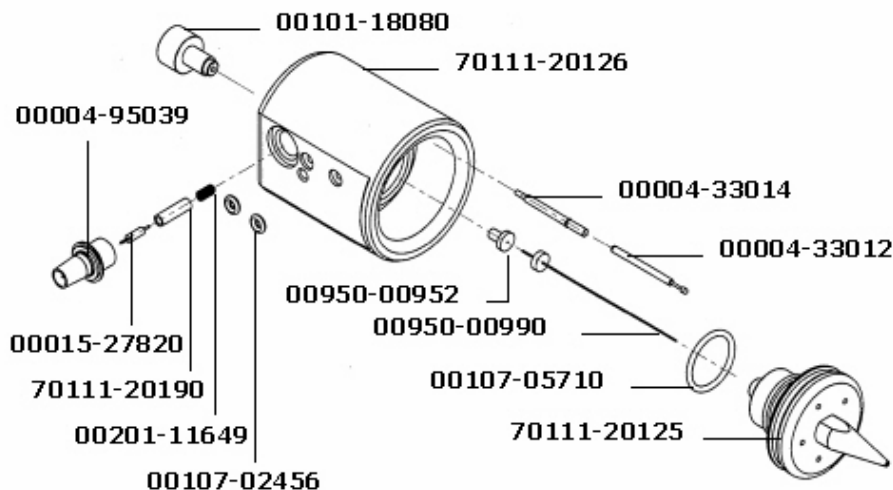


Figure 8-1. ESI probe part numbers

APCI Source

Housing, APCI Assembly	OPTON-20002
Probe, APCI.....	70111-60078
Screw, PN, Phillips, 4-40 × 1/4 in., stainless steel	00405-44007
Washer, flat #4, 0.312 in. OD × 0.03 in. ID, stainless steel	00470-00410
Vaporizer Assembly, APCI Probe	70111-60040S
Position Adjustor Assembly, APCI Probe.....	70111-60077
Vaporizer Assembly, APCI Probe	70111-60040S
Ferrule, 0.016 in. ID, PEEK, HPLC.....	00101-18120
Fitting, Fingertight 2, Upchurch Scientific®	00101-18195
Ferrule, Fingertight 2, Upchurch.....	00101-18196
Fitting, flangeless, 1/8 in, green, Upchurch	00101-18198
Fitting, ferrule, 1/8 in, Tefzel® (2 each).....	00101-18199
Fitting, flangeless, 1/8 in, blue, Upchurch	00101-18200
Tubing, fused-silica, 0.150 mm ID × 0.363 mm OD	00106-10498
O-ring, 0.239 in. ID × 1/16 in., Viton.....	00107-04000
Manifold, APCI.....	70005-20201
Fitting, 10-32 male, nut, PEEK	70005-20220
Fitting, APCI, flange	70005-20250
O-ring, 0.185 in. ID × 0.056 in., Viton (2 each).....	00107-02585
O-ring, 0.614 in. ID × 1/16 in., Viton.....	00107-05700
O-ring, 0.625 in. ID × 0.029 in., Viton.....	00107-09015
Screw, pan head, SLT, 4-40 × 3/16 in., stainless steel.....	00414-44005
Screw, socket, 4-40 × 3/16 in., Ag plated	00419-44005
Washer, flat, #4, 0.312OD × 0.03 in., stainless steel.....	00470-00410
Tube, vaporizer, APCI.....	70005-20194
Insulator, heater, APCI	70005-20195
Nozzle, APCI	70005-20196
Tube, auxiliary, Gas, APCI	70005-20199
Tube, sheath gas, APCI	70005-20200
Heater coil, APCI	70005-20216
Vaporizer casing, APCI	70005-20217
Retainer, heater, APCI.....	70111-20270
Assembly, flange, vaporizer, APCI	70111-60039

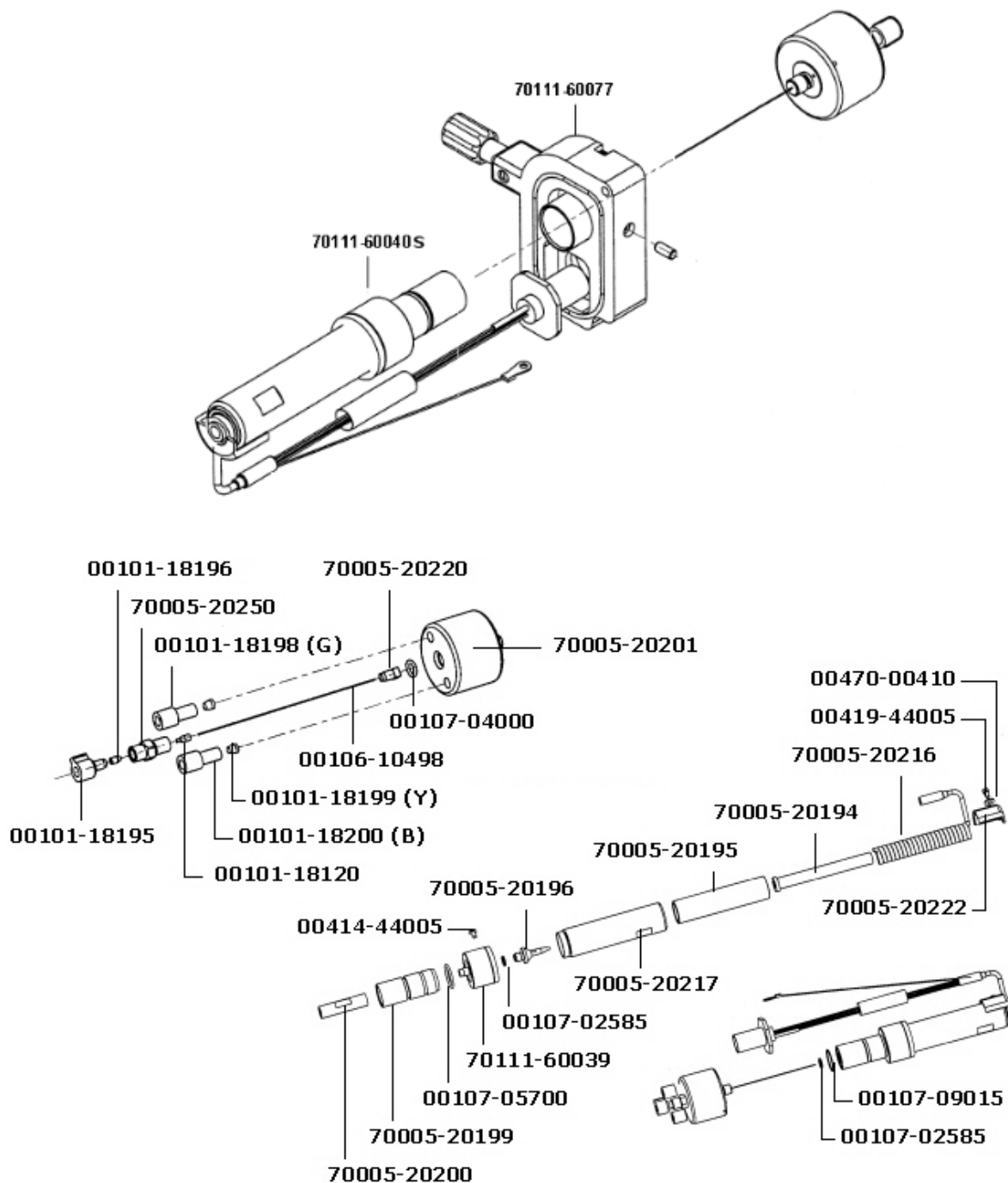


Figure 8-2. APCI probe and vaporizer assembly part numbers

Ion Source Interface

O-ring, 0.3 in. ID × 0.064 in., Kalrez, CMPD, 4079	00107-12750
Ion transfer tube, 65 × 0.5 in. ID	70111-20100
Shield, sweep spray.....	70111-20245
Shield, sample spray (Ion sweep cone).....	70111-20305

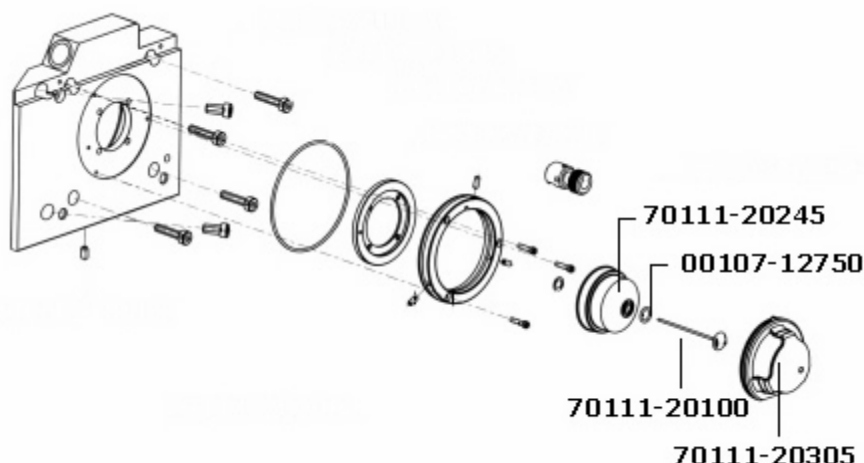


Figure 8-3. Ion source interface part numbers

Divert/Inject Valve

Divert/inject valve, Rheodyne 7750E-185.....	70111-98005
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Syringe Pump

Syringe pump	97033-98020
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Forepump

TSQ Quantum Mechanical Pump Kit	70111-62014
Vacuum hardware clamp KF-20/25.....	00102-10020
Pump hardware centering ring	00108-02011
Mechanical pump 650L/ME2M30 220V ac.....	00108-02655
Hose clamp, band	00201-03810
PVC vacuum hose, reinforced.....	00301-24163
Tool, Extraction, Minifit.....	00725-00050
Adapter, pump roughing line.....	70111-20210
Mist filter	00108-02-00002
Drain oil return kit.....	00960-01-00007

8.2 Data System Hardware

Data system computer	70111-62018
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8.3 Manuals

Finnigan TSQ Quantum Preinstallation Requirements Guide	70111-97040
Finnigan TSQ Quantum Getting Connected	70111-97041
Finnigan TSQ Quantum Getting Started	70111-97042
Finnigan TSQ Quantum Hardware Manual	70111-97043

8.4 Accessory Kit

Accessory Kit	70111-62008
Fuse, 1/8 A, 250 V	00006-01604
Fuse 0.1 A, 250 V	00006-07005
Fuse, 1.6 A, 250 V	00006-08600
Fuse, 2 A, 250 V (Analyzer Control PCB fuse F7)	00006-09102
Fuse, 2 A, 250 V (Interlock PCB fuses F1 and F3)	00006-10510
Fuse, 4 A, 250 V (Source PCB fuse F3)	00006-11420
Fuse, 6.3 A, 250 V (Interlock PCB fuses F2 and F4)	00006-11450
Fuse 10 A, 250 V (Analyzer Control PCB fuses F4 and F5)	00006-14015
Tool, Hex ball driver, 3/16 in.	00025-01700
Tool, Hex ball driver, 7/64 in.	00025-01800
Tool, Hex ball driver, 5/32 in., 7.4 in. long	00025-10020
Fitting, ferrule, Swagelok, Back, 1/8 in. (2 each)	00101-02500
Fitting, ferrule, Swagelok, Back, 1/4 in. (2 each)	00101-04000
Fitting, ferrule, Swagelok, Front, 1/8 in. (2 each)	00101-08500
Fitting, ferrule, Swagelok, Front, 1/4 in. (2 each)	00101-10000
Fitting, Swagelok, Nut, 1/4 in., brass	00101-12500
Fitting, Swagelok, Nut, 1/8 in., brass (2 each)	00101-15500
Fitting, nut, HPLC, Fingertight (2 each)	00101-18081
Ferrule, 0.008 in. ID, KEL-F, HPLC (4 each)	00101-18114
Ferrule, 0.016 in. ID, PEEK, HPLC (4 each)	00101-18120
Fitting, Fingertight 2, Upchurch	00101-18195
Ferrule, Fingertight 2, Upchurch (3 each)	00101-18196
Fitting, flangeless, 1/8 in. Upchurch	00101-18198
Fitting, ferrule, 1/8 in. Tefzel	00101-18199
Fitting, flangeless, 1/8 in. Blue Delrin	00101-18200
Fitting, HPLC Union, 0.010 orifice, PEEK	00101-18202
Fitting, HPLC, Tee, 0.020 orifice, PEEK	00101-18204
Tubing, fused silica, 0.150 mm × 0.390 mm	00106-10498
Tubing, fused silica, 0.10 mm ID × 0.19 mm OD	00106-10499

Tubing, fused silica, 0.05 mm ID × 0.19 mm OD, deactivated	00106-10502
Tubing, fused silica, 0.11 mm ID × 0.4 mm OD, deactivated.....	00106-10504
Tubing, fused silica, 75 microns	00106-10511
Tube, Hypodermic 28 gauge × 10 in., 304 stainless steel.....	00106-20000
O-ring, 0.3 in. ID × 0.064 in., Kalrez, CMPD, 4079	00107-12750
Sample loop, Rheodyne HPLC, 5 µL.....	00110-22026
Sample loop, Rheodyne HPLC, 20 µL.....	00110-22028
Rheodyne Needle Port.....	00110-22030
Chemical, reserpine	00301-12901
Syringe, 250 µL, 2-in needle, 22 gauge, type S	00301-19006
Syringe, 10 µL, Rheodyne	00301-19008
Syringe, 250 µL, Gas Tight, Removable needle	00301-19015
Syringe, 500 µL, Gas Tight, Removable needle	00301-19016
Tubing, PEEK, 0.005 ID × 1/16 in. OD, Red, 5 ft. (1.5 m long)	00301-22912
Tubing, Teflon, 0.030 in. ID × 1/16 in. OD	00301-22915
Polytyrosine-1,3,6 Tuning and Calibration Solution (liquid).....	00301-22924
Polytyrosine-1,3,6 Tuning and Calibration Solution (solid)	00301-22925
Tool, Ball driver, Allen-Hex, 3/32.....	00725-00030
Wrench, L, hex, 4 mm	00725-00034
Tool, Hex ball driver, 3.0 mm	00725-00055
Tool, Screwdriver, Phillips, 10 in., No 2	00725-00070
Tool, Driver, T-Hex, 7/64, 12 in.	00725-00100
Seal, STD, Needle, 5000 Series	00950-00952
Needle, D Point, 26 gauge, 2 in. long, 0.24D washer	00950-00990
Syringe Adapter Kit	70005-62011
Needle, Corona, APCI.....	70005-98033
Ion transfer tube, insert, replaceable	70111-20100
Tool, ion transfer tube removal	70111-20258
Kit, Metal Needle, 32-gauge	OPTON-20004
Kit, Metal Needle, 34-gauge	OPTON-20005
Kit, polytyrosine, vial.....	70111-62021

8.5 Metal Needle Kits

High Flow Needle Kit..... **OPTON-20004**

(Recommended for LC flow rates between 5 and 400 $\mu\text{L}/\text{min}$)

Ferrule, 0.008 in. ID, Kel-F	00101-18114
Ferrule, 0.012 in. ID, Kel-F	00101-18116
Fitting, Fingertight 2, Upchurch	00101-18195
Union, zero dead volume, 1/4-28, Upchurch.....	70111-20233
Blunt-tip, 32-gauge, 50 μm ID, stainless steel needle	70111-20287

Low Flow Metal Needle Kit..... **OPTON-20005**

(Recommended for LC flow rates between 500 nL/min and 10 $\mu\text{L}/\text{min}$)

Ferrule, 0.012 in. ID, Kel-F	00101-18114
Ferrule, 0.012 in. ID, Kel-F	00101-18116
Fitting, Fingertight 2, Upchurch	00101-18195
Union, zero dead volume, 1/4-28, Upchurch.....	70111-20233
Blunt-tip, 34-gauge, 30 μm ID, stainless steel needle	70111-20288

8.6 Fittings, Ferrules, and Sample Loops

Ferrule, Fingertight 2, Upchurch. (for: PEEK tubing and Teflon tube)	00101-18196
Ferrule, 0.016 in. ID, PEEK, Upchurch (for: Fused-silica capillary infusion line)	00101-18120
Ferrule, 0.012 in. ID, Kel-F, Upchurch (for: High and low flow metal needles).....	00101-18114
Ferrule, 0.008 in. ID, Kel-F, Upchurch (for: Fused-silica capillary sample line).	00101-18116
Ferrule, LC, 1/16 in., stainless steel, Rheodyne	2522-3830
Fitting, Fingertight, Upchurch.....	00101-18195
Fitting, Fingertight, Upchurch.....	00101-18081
Fitting, adapter, Kel-F, 10-32 \times 1/4-28, Upchurch (connects to ESI probe inlet).....	00101-18080
Nut, LC, 1/16 in., stainless steel, Rheodyne.	2522-0066
Fitting, LC union, 0.010 in. orifice, PEEK.	00101-18202
Fitting, LC TEE union, 0.020 in. orifice, PEEK	00101-18204
Fitting, adapter union, PEEK, Upchurch.....	00101-18206
5 μL sample loop, stainless steel.....	00110-22026
10 μL sample loop, stainless steel.....	00110-22012
20 μL sample loop, stainless steel.....	00110-22028
50 μL sample loop, stainless steel.....	00110-22016
100 μL sample loop, stainless steel.....	00110-22018
500 μL sample loop, stainless steel.....	00110-22020
1 mL sample loop, stainless steel.	00110-22022

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