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# **Orbitrap Exploris Series**

Orbitrap Exploris 120, Orbitrap Exploris 240, Orbitrap Exploris 480, and Orbitrap Exploris MX

## **Operating Manual**

BRE0014471 Revision E October 2021



# **Orbitrap Exploris Series**

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#### General Lab Equipment, Not for Clinical, Patient or Diagnostic Use.

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# **Technical Data for Orbitrap Exploris 120, Orbitrap Exploris 240, and Orbitrap Exploris MX Systems**

The table summarizes the most important technical data of these systems. See the respective chapters of the manual for details and additional instrument properties.

Technical Data for Orbitrap Exploris 120, Orbitrap Exploris 240, and Orbitrap Exploris MX Systems (Sheet 1 of 2)

Parameter	Specifica	tion	Value
Instrument Properties			
Mass spectrometer	Length × width × height		763 × 534 × 703 mm
	Weight		120 kg
Forepump <sup>a</sup>	Length >	« width × height	530 × 330 × 360 mm
	Weight		60 kg
Complete system	Noise en	nission	Below 70 dB(A)
(incl. data system)	Heat ger	neration	2350 W
Power Requirements			
Mass spectrometer	Input	Nominal voltage	208–240 V AC, 50/60 Hz, 10 A
		Power	apparent power: 800 VA; effective power: 750 W
		Fuse <sup>b</sup>	15/16 A (tripping characteristic C)
	Output	4×	208–240 V AC, 50/60 Hz, 3 A total
	Degree of protection		IP20
	Protection class		Class I
	Overvoltage category		II
Forepump	Input	Nominal voltage	200–240 V AC, 50/60 Hz
		Power	1.5 kW
		Fuse <sup>b</sup>	15/16 A (tripping characteristic C)
Data system	Input	Nominal voltage	100–240 V AC, 50/60 Hz
		Fuse	15/16 A
Gas Requirements			
Source gas	Туре		Nitrogen
(minimum	Purity		99% or better (high purity)
requirement)	Supply rate		max. 45 ln/min
	Pressure		0.6 ± 0.05 MPa
HCD gas / reagent	Туре		Nitrogen
carrier gas	Purity		99.999% or better (ultra high purity)
(mandatory)	Supply r	ate	max. 0.03 ln/min <sup>c</sup>
	Pressure		0.6 ± 0.05 MPa

Parameter	Specification	Value
Operating Environment		
	Laboratory temperature	18–27 °C
	Max. temperature	0.5 °C/10 min
	fluctuation	
	Humidity	20–80%, non-condensing and non-corrosive atmosphere
	Pollution degree	2
	Max. altitude	3000 m above sea level
Pump exhaust	Inrush flow rate	10 L/min
requirements	Continuous flow rate	7 L/min
Ion source exhaust requirements	Maximum flow rate	45 L/min

Technical Data for Orbitrap Exploris 120, Orbitrap Exploris 240, and Orbitrap Exploris MX Systems (Sheet 2 of 2)

<sup>a</sup> Leybold SOGEVAC<sup>™</sup> SV 65 BI, or approved equivalent model. Values depend on the actually used pump model.

<sup>b</sup> dedicated wall outlet

 $^{\rm c}$  With the Internal Calibration source in use, the consumption of UHP nitrogen increases up to 65 sccm (»0.07 ln/min).

# **Technical Data for Orbitrap Exploris 480 Systems**

The table summarizes the most important technical data of the system. See the respective chapters of the manual for details and additional instrument properties.

Parameter	Specifica	tion	Value
Instrument Properties			
Mass spectrometer	Length >	« width × height	763 × 534 × 703 mm
	Weight		120 kg
Source vacuum pump <sup>a</sup>	Length >	< width × height	731 × 420 × 490 mm
	Weight		82 kg
Auxiliary forepump <sup>b</sup>	Length >	< width × height	411 × 127 × 191 mm
	Weight		17 kg
Complete system	Noise en	nission	Below 70 dB(A)
(incl. data system)	Heat ger	neration	2650 W
Power Requirements			
Mass spectrometer	Input	Nominal voltage	208–240 V AC, 50/60 Hz, 10 A
		Power	apparent power: 800 VA; effective power: 750 W
		Fuse <sup>c</sup>	15/16 A (tripping characteristic C)
	Output	4×	208–240 V AC, 50/60 Hz, 3 A total
	Degree of protection		IP20
	Protection class		Class I
	Overvoltage category		II
Source vacuum pump	Input	Nominal voltage	200–240 V AC, 50/60 Hz
		Power	2.2 kW
		Fuse <sup>c</sup>	15/16 A (tripping characteristic C)
Auxiliary forepump	Input	Nominal voltage	115 V or 230 V AC, 50/60 Hz, single phase
		Power	0.25 kW (50 Hz) / 0.3 kW (60 Hz)
		Fuse <sup>c</sup>	16 A (115 V) / 6 A (230 V), slow
Data system	Input	Nominal voltage	100–240 V AC, 50/60 Hz
		Fuse	15/16 A

Technical Data for Orbitrap Exploris 480 Systems (Sheet 1 of 2)

Parameter	Specification	Value
Gas Requirements		
Source gas	Туре	Nitrogen
(minimum	Purity	99% or better (high purity)
requirement)	Supply rate	max. 45 ln/min
	Pressure	0.6 ± 0.05 MPa
HCD gas (mandatory)	Туре	Nitrogen
	Purity	99.999% or better (ultra high purity)
	Supply rate	max. 0.03 ln/min <sup>d</sup>
	Pressure	0.6 ± 0.05 MPa
Operating Environment		
	Laboratory temperature	18–27 °C
	Max. temperature	0.5 °C/10 min
	fluctuation	
	Humidity	20-80%, non-condensing and non-corrosive atmosphere
	Pollution degree	2
	Max. altitude	3000 m above sea level
Pump exhaust	Inrush flow rate	10 L/min
requirements	Continuous flow rate	7 L/min
Ion source exhaust requirements	Maximum flow rate	45 L/min

Technical Data for Orbitrap Exploris 480 Systems (Sheet 2 of 2)

<sup>a</sup> Leybold SOGEVAC<sup>™</sup> SV 120 BI, or approved equivalent model. Values depend on the actually used pump model.
 <sup>b</sup> Pfeiffer DUO 11, or approved equivalent model. Values depend on the actually used pump model.

<sup>c</sup> dedicated wall outlet

<sup>d</sup> With the Internal Calibration source in use, the consumption of HCD collision gas increases up to 65 sccm ( $\approx$ 0.07 ln/min).

# **Using this Manual**

Welcome to the Thermo Scientific<sup>™</sup> Orbitrap Exploris Series system! Orbitrap Exploris Series systems are members of the Thermo Scientific family of mass spectrometers that are powered by Orbitrap<sup>™</sup> technology.

#### Contents

- About this Manual on page 1-1
- Typographical Conventions on page 1-2
- Reference Documentation on page 1-4
- Contacting Us on page 1-5

## **About this Manual**

This Orbitrap Exploris Series Operating Manual contains precautionary statements that can prevent personal injury, instrument damage, and loss of data if properly followed. It also describes the modes of operation and principle hardware components of your Orbitrap Exploris Series instrument. In addition, this manual provides step-by-step instructions for cleaning and maintaining your instrument.

Designed, manufactured and tested in an ISO9001 certified facility, this instrument has been shipped to you from our manufacturing facility in a safe condition. This instrument must be used as described in this manual. Any use of this instrument in a manner other than described here may result in instrument damage and/or operator injury.

## **Typographical Conventions**

	This section describes typographical conventions that have been established for Thermo Fisher Scientific manuals.
Signal Words	
	Make sure that you follow the precautionary statements presented in this manual. The special notices appear different from the main flow of text:
NOTICE	Points out possible damage to instrument and material, and other important information in connection with the instrument.
	<b>Tip</b> Highlights helpful information that can make a task easier.
Viewpoint Orientation	
	The expressions <i>left</i> and <i>right</i> used in this manual always refer to the viewpoint of a person that is facing the front side of the instrument.
Data Input	
	Throughout this manual, the following conventions indicate data input and output with the computer:
	• Messages displayed on the screen are represented by capitalizing the initial letter of each word and by italicizing each word.
	• Input that you enter by keyboard is identified by quotation marks: single quotes for single characters, double quotes for strings.
	• For brevity, expressions such as "choose <b>File &gt; Directories</b> " are used rather than "pull down the File menu and choose Directories."
	<ul> <li>Any command enclosed in angle brackets &lt; &gt; represents a single keystroke. For example, "press <f1>" means press the key labeled <i>F1</i>.</f1></li> </ul>
	• Any command that requires pressing two or more keys simultaneously is shown with a plus sign connecting the keys. For example, "press <b><shift></shift></b> + <b><f1></f1></b> " means press and hold the <b><shift></shift></b> key and then press the <b><f1></f1></b> key.
	• Any button that you click on the screen is represented in bold face letters. For example, "click <b>Close</b> ."

## **Topic Headings**

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

# **Chapter Name**

## **Second Level Topics**

**Third Level Topics** 

**Fourth Level Topics** 

## **Reference Documentation**

This Orbitrap Exploris Series Operating Manual represents the Original Operating Instructions. In addition to this manual, Thermo Fisher Scientific provides other documents for the Orbitrap Exploris Series mass spectrometer that are not part of the Original Operating Instructions. Reference documentation for the Orbitrap Exploris Series MS includes the following:

• Orbitrap Exploris Series Pre-Installation Requirements Guide

This manual contains information on the necessary environmental conditions in the intended location for the instrument.

• Orbitrap Exploris Performance Maintenance Manual

This manual describes the user maintenance for the quadrupole and the bent flatapole.

- *Orbitrap Exploris 120 Software Manual* (with Orbitrap Exploris 120 system)
- *Orbitrap Exploris 240 Software Manual* (with Orbitrap Exploris 240 system)
- *Orbitrap Exploris 480 Software Manual* (with Orbitrap Exploris 480 system)
- *Orbitrap Exploris MX Software Manual* (with Orbitrap Exploris MX system)

You can access PDF files of the documents listed above and of this manual from the data system computer.

#### ✤ To view product manuals

From the Microsoft<sup>™</sup> Windows<sup>™</sup> task bar, choose **Start > All Programs > Thermo Instruments > model x.x**, and then open the applicable PDF file.

Refer also to the user documentation that is provided by the manufacturers of third-party components:

- Forepumps
- Turbomolecular pump
- Syringe pump
- Data system computer and monitor
- Safety data sheets

## **Contacting Us**

There are several ways to contact Thermo Fisher Scientific. You can use your smartphone to scan a QR Code, which opens your email application or browser.

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Patent Information	Your Thermo Scientific product may be manufactured under or covered by at least one or more U.S. patents and other patents pending. See www.thermofisher.com/patents for details.	
Service Contact	For technical support related to your instrument or software, visit the <b>Services &amp; Support</b> tab at www.thermofisher.com or visit www.unitylabservices.com to find the customer care telephone line or email address for your geographical region.	
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Customer Feedback	<ul> <li>To suggest changes to this manual</li> <li>You are encouraged to report errors or omissions in the text or index. Send an email to the Technical Documentation at documentation.bremen@thermofisher.com.</li> <li>The PDF versions of our manuals allow adding comments with Adobe Acrobat Reader or other freely available PDF reader programs.</li> </ul>	

Using this Manual Contacting Us

# **Scope of Delivery**

This chapter lists the components that are shipped with your Orbitrap Exploris Series mass spectrometer.

The Orbitrap Exploris Series standard system has the following components:

- Orbitrap Exploris Series mass spectrometer
- API Source with HESI probe
- Calibration ESI probe
- Data system computer with monitor
- Depending on the instrument type:
  - one forepump (Orbitrap Exploris 120 MS, Orbitrap Exploris 240 MS. and Orbitrap Exploris MX MS), or
  - two forepumps (Orbitrap Exploris 480 MS)<sup>1</sup>
- Noise reduction covers and drip pans for forepumps
- Syringe pump
- Installation Kit including
  - Equipment for connecting the above components (hoses, cables)
  - Computer equipment
  - Tools for installation and maintenance
  - Spare parts

<sup>&</sup>lt;sup>1</sup> One pump in case of the dry pump option. See page 5-8,

**Scope of Delivery** 

# **Functional Description**

This chapter describes the principal components of the Orbitrap Exploris Series mass spectrometers and their respective functions.

#### Contents

- General Description on page 3-2
- Instrument Front Side on page 3-9
- Left Instrument Side on page 3-17
- Right Instrument Side on page 3-20
- Ion Optics on page 3-26
- Curved Linear Trap on page 3-32
- Ion-Routing Multipole on page 3-33
- Orbitrap Analyzer on page 3-34
- Vacuum System on page 3-37
- Electronic Assemblies on page 3-40
- Cooling Fans on page 3-40
- Additional Hardware on page 3-41

## **General Description**

The Orbitrap Exploris Series mass spectrometers are stand-alone Orbitrap<sup>™</sup> instruments with an atmospheric pressure ionization (API) source for liquid chromatography (LC) mass spectrometry (MS) high-throughput applications. The instruments are designed to be placed on a bench in the laboratory.

The Orbitrap Exploris Series comprises these instruments:

- Orbitrap Exploris 120 MS
- Orbitrap Exploris 240 MS
- Orbitrap Exploris 480 MS
- Orbitrap Exploris MX MS

#### Layout of the Orbitrap Exploris Series Mass Spectrometers



Figure 3-1. Orbitrap Exploris 480 MS with Vanquish HPLC

The Orbitrap Exploris Series mass spectrometers consists of the following main components. They are described in the topics that follow:

- Ion source
- Thermo Scientific<sup>™</sup> EASY-IC<sup>™</sup> ion source for improved mass-to-charge ratio (*m/z*) assignment
- Injection filter with mass resolving capabilities
- Quadrupole mass filter for precursor ion selection

In the Orbitrap Exploris MX MS, a transfer quadrupole replaces the quadrupole.

• Ion-routing multipole for trapping ions and performing HCD (Higher Energy Collisional Dissociation) experiments

HCD experiments are not available for the Orbitrap Exploris MX MS.

- Intermediate storage device (C-Trap) for short pulse injection
- Orbitrap analyzer for Fourier transform mass analysis

For a schematic of the instrument layout, see Figure 3-15 on page 3-26. Figure 3-1 shows a front view of the Orbitrap Exploris 480 MS.

### **Operating Modes of the Orbitrap Exploris Series Mass Spectrometers**

The samples can be introduced into the Thermo Scientific OptaMax NG<sup>™</sup> API source at the front side by a variety of methods that include direct infusion (with a syringe pump) or a U-HPLC system (for example, Thermo Scientific UltiMate 3000). See "Atmospheric Pressure Ionization Source" on page 3-10 for details.

The IC source delivers calibrant ions into the stream of analyte ions. The instrument software uses the precisely known mass-to-charge ratio of the calibration mass peak to fine-adjust the instrument's mass-to-charge ratio calibration. See "Internal Calibrant Discharge Source" on page 3-28 for details.

The injection filter transmits the ions from the source to the quadrupole or transfer quadrupole. The injection filter also performs coarse pre-filtering of the ions according to their mass-to-charge ratios. See page 3-30 for details.

For the Orbitrap Exploris 120, Orbitrap Exploris 240, and Orbitrap Exploris 480 MSs, the quadrupole rod assembly operates as an ion transmission device with the possibility to filter the transmitted ions according to their mass-to-charge ratios. By applying RF voltages and DC voltages to the rods, the filter characteristic is configured. See "Quadrupole Mass Filter" on page 3-30 for details.

For the Orbitrap Exploris MX MS, the transfer quadrupole guides the ions towards the C-Trap.

The ions are transferred into the C-Trap through four stages of differential pumping. See "Ion Optics" on page 3-26 for details. The ions are passed through the C-Trap into the ion-routing multipole (IRM). See page 3-33 for a description of the IRM.

For the Orbitrap Exploris 120, Orbitrap Exploris 240, and Orbitrap Exploris 480 MSs, the IRM adds a Higher Energy Collision Induced Dissociation capability to the instrument. In combination with the quadrupole mass filter, this allows MS/MS experiments or all-ion fragmentation (AIF) in case of a broad range of selected mass-to-charge ratios. After the ions have been fragmented in the IRM, the IRM

voltages are ramped up and the ions are transferred back into the C-Trap.

For the Orbitrap Exploris MX MS, the ions are cooled and trapped in the IRM. Then, the IRM voltages are ramped up and the ions are transferred back into the C-Trap. See page 3-33 for a description of the IRM.

From the C-Trap, the ions are then injected through three further stages of differential pumping by a lens system (Z-lens) into the Orbitrap analyzer where mass spectra are acquired by image current detection. The vacuum inside the Orbitrap analyzer is maintained below 1E-9 mbar. See "Orbitrap Analyzer" on page 3-34 for details.

## Performance Specifications of Orbitrap Exploris Series Mass Spectrometers

Mass Range for Full Scans	<ul> <li>m/z 40-3000</li> <li>The following mass range limitations apply:</li> <li>If first mass is ≥ m/z 150, set last mass ≤ 15× first mass.</li> <li>If first mass is 50 ≤ m/z &lt; 150, set last mass ≤ 10× first mass.</li> </ul>				
	• If first mass is $40 < m/z < 50$ , set last mass $\le 5 \times$ first mass.				
Precursor Ion Selection	Recommended isolation width $[m/z]$ for a given precursor with $m/z$ x:				
<i>m/z</i> range	Minimum	Maximum			
$40 < x \le 400$	0.4				
$400 < x \le \qquad 700$	0.7	SIM. 50			
$700 < x \le 1000$	1.0	MS/MS: 5			
$1000 < x \le 1500$	1.5	1013/1013. )			
$1500 < x \le 2000$	2.0				
$2000 < x \leq  3000$	No precursor ion selection				
Mass Resolution	15000 at <i>m/z</i> 200 at a scan rate of 22 Hz				
	30000 at $m/z$ 200 at a scan rate of 12 Hz				
	60000 at <i>m/z</i> 200 at a scan rate of 7 Hz				
	120000 at $m/z$ 200 at a scan rate o	f 3 Hz			
Mass Accuracy	<3 ppm with external calibration (under defined conditions) <1 ppm using internal standard, lock masses (under defined conditions)				
Polarity Switching	One full cycle in >1.4 sec (one full scan positive mode and one full scar negative mode at resolution setting of 60000)				
Dynamic Range	>5000 within a single scan				
Sensitivity	MS/MS: 200 fg reserpine on column tSIM: 200 fg reserpine on column S/	n S/N 100:1 /N 250:1			

<b>Table 3-1.</b> Performance specifications of the Urbitrap Exploris 120 N	ЛS
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Mass Range for Full Scans $m/z 40-6000 (8000 \text{ with BioPharma option})$ The following mass range limitations apply: • If first mass is $\geq m/z 150$ , set last mass $\leq 15 \times$ first mass. • If first mass is $50 \leq m/z < 150$ , set last mass $\leq 10 \times$ first mass. • If first mass is $40 < m/z < 50$ , set last mass $\leq 5 \times$ first mass.Preserves len SelectionDescent of the last is $10 \times 10^{-6}$ ( $10 \times 10^{-6}$ )		a option) s apply: t mass $\leq 15 \times$ first mass. et last mass $\leq 10 \times$ first mass. last mass $\leq 5 \times$ first mass.	
Precursor Ion Selection	Recommended isolation width $\lfloor m/z \rfloor$ for a given precursor with $m/z$ x:		
<i>m/z</i> range	Minimum	Maximum	
$40 < x \le 400$	0.4		
$400 < x \le 700$	0.7		
$700 < x \le 1000$	1.0	SIM: 50	
$1000 < x \le 1500$	1.5	MS/MS: 5	
$1500 < x \le 2000$	2.0		
$2000 < x \le 2500$	3.0		
$2500 < x \le 6000  (8000)$	No precursor ion selection		
Mass Resolution	15000 at <i>m/z</i> 200 at a scan rate o	f 22 Hz	
	30000 at $m/z$ 200 at a scan rate of 12 Hz		
	45000 at $m/z$ 200 at a scan rate of 10 Hz		
	60000 at $m/z200$ at a scan rate of	f 7 Hz	
	120000 at $m/z$ 200 at a scan rate of	f 3 Hz	
	180000 at $m/z 200$ at a scan rate of	f 2 Hz	
	240000 at $m/z200$ at a scan rate of	f 1.5 Hz	
Mass Accuracy	<3 ppm with external calibration (under defined conditions)		
	<1 ppm using internal standard, lock masses (under defined condit		
Polarity SwitchingOne full cycle in >1.4 sec (one full scan positive mode and one full negative mode at resolution setting of 60000)		can positive mode and one full scan of 60 000)	
Dynamic Range>5000 within a single scan			
SensitivityMS/MS: 200 fg reserpine on column S/N 100:1SIM: 200 fg reserpine on column S/N 250:1		n S/N 100:1 N 250:1	

## **Table 3-2.**Performance specifications of the Orbitrap Exploris 240 MS

Mass Range for Full Scans	<ul> <li>m/z 40-6000 (8000 with BioPharma option) The following mass range limitations apply:</li> <li>If first mass is ≥ m/z 150, set last mass ≤ 15× first mass.</li> <li>If first mass is 50 ≤ m/z &lt; 150, set last mass ≤ 10× first mass.</li> <li>If first mass is 40 &lt; m/z &lt; 50, set last mass ≤ 5× first mass.</li> </ul>	
Precursor Ion Selection	Recommended isolation width $[m/z]$ for a given precursor with $m/z$ x:	
<i>m/z</i> range	Minimum	Maximum
$40 < x \le 400$	0.4	
$400 < x \le 700$	0.7	
$700 < x \le 1000$	1.0	< <b>y</b>
$1000 < x \le 1500$	1.5	NA NA
$1500 < x \le 2000$	2.0	
$2000 < x \le 2500$	3.0	
$2500 < x \le 6000  (8000)$	No prec	cursor ion selection
Mass Resolution	7500 at <i>m/z</i> 200 at a scan r	ate of 40 Hz
	$15000 \text{ at } m/z \ 200 \text{ at a scan r}$	ate of 22 Hz
	$30000 \text{ at } m/z \ 200 \text{ at a scan r}$	ate of 12 Hz
	45000 at $m/z$ 200 at a scan r	ate of 10 Hz
	60000 at <i>m</i> / <i>z</i> 200 at a scan r	ate of 7 Hz
	$120000 \text{ at } m/z \ 200 \text{ at a scan r}$	ate of 3 Hz
	$180000 \text{ at } m/z \ 200 \text{ at a scan r}$	ate of 2 Hz
	240000 at $m/z200$ at a scan r	ate of 1.5 Hz
	$480000 \text{ at } m/z \ 200 \text{ at a scan r}$	ate of 0.7 Hz
Mass Accuracy	<3 ppm with external calibration (under defined conditions) <1 ppm using internal standard, lock masses (under defined conditions)	
Polarity Switching	olarity Switching One full cycle in >1.4 sec (one full scan positive mode and one full s negative mode at resolution setting of 60000)	
Dynamic Range	vnamic Range     >5000 within a single scan	
Sensitivity	MS/MS: 50 fg reserpine on colu SIM: 50 fg reserpine on column	ımn S/N 100:1 1 S/N 150:1

**Table 3-3.**Performance specifications of the Orbitrap Exploris 480 MS

Table 3-4.	Performance specifications of the Orbitrap Exploris MX MS
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Mass Range for Full Scans	<ul> <li>m/z 40-3000 (8000 with BioPharma option) The following mass range limitations apply:</li> <li>If first mass is ≥ m/z 150, set last mass ≤ 15× first mass.</li> <li>If first mass is 50 ≤ m/z &lt; 150, set last mass ≤ 10× first mass.</li> <li>If first mass is 40 &lt; m/z &lt; 50, set last mass ≤ 5× first mass.</li> </ul>	
Mass Resolution	Last mass - First Mass > 50 15000 at $m/z$ 200 at a scan rate of 22 Hz 30000 at $m/z$ 200 at a scan rate of 12 Hz 60000 at $m/z$ 200 at a scan rate of 7 Hz 120000 at $m/z$ 200 at a scan rate of 3 Hz 180000 at $m/z$ 200 at a scan rate of 2 Hz	
Mass Accuracy	<3 ppm with external calibration (under defined conditions) <1 ppm using internal standard, lock masses (under defined conditions)	
Polarity Switching	One full cycle in >1.4 sec (one full scan positive mode and one full scan negative mode at resolution setting of 60000)	
Dynamic Range	>5000 within a single scan	

## **Instrument Front Side**

System status control LEDs and API source are at the front side of the instrument.

## **System Status LEDs**

Three system status LEDs at the front side (see Figure 3-2) indicate the main functions of the system. Table 3-5 explains the function of the LEDs.

alus	Scan

Figure 3-2. System status LEDs

<b>Table 3-5.</b> System status LEDs of the Orbitrap Exploris Series mass spece
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LED	Status	Information		
Power	Green	Instrument is receiving power. (The electronics service switch is in the Operating Mode position.)		
	Off	Instrument is not receiving power.		
Status	tus Green Instrument is in operating mode.			
	White flashing	Procedure in progress		
Yellow Warn status, does no affected.		Warn status, does not prevent measurement, but proper operation could be affected.		
	Yellow flashing	Grave failure detected that does prevent measurement.		
	Off	The electronics service switch is in the Service Mode position. Pumps are running but electronics is switched off.		
Scan	Blue animation <sup>a</sup>	Instrument is scanning in MS1 mode.		
	Purple animation	Instrument is scanning in MS2 mode.		
	White bar graph	Progress bar for procedure.		
	Same as Status LED (in Standby Mode)	Same as Status LED.		
	Off	Instrument is powered but in off mode.		

**Tip** The system status LEDs give a overview of the general system status. They do not have any function for the safety status of the instrument. It is not sufficient that the Power LED is off because it might be defective. Before you perform any maintenance on the instrument, make sure that the main power circuit breaker switch (labeled Main Power) is in the Off (O) position and that the power cords of the *mass spectrometer and the forepumps* are disconnected.

<sup>a</sup> The animation changes with the actual scan rate.

## **Atmospheric Pressure Ionization Source**

The atmospheric pressure ionization (API) source forms gas-phase sample ions from sample molecules that are contained in solution. The API source also serves as the interface between the LC and the mass spectrometer. The Orbitrap Exploris Series mass spectrometer is shipped with the Thermo Scientific OptaMax NG<sup>™</sup> API source and a HESI probe. See Figure 3-3.



Figure 3-3. API source with HESI probe attached

#### **API Source**

The API source is the part of the ion source that is at atmospheric pressure. You can configure the API source to operate in any of several API modes, including heated electrospray ionization (HESI), atmospheric pressure chemical ionization (APCI), and atmospheric pressure photoionization (APPI). For APCI and APPI, additional parts are required. See Figure 3-4. A separate nanospray ionization (NSI) probe is necessary to operate in NSI mode. The ions produced in the API source are transmitted by the ion optics into the Orbitrap mass analyzer, where they are separated according to their mass-to-charge ratios.

The API source housing enables you to quickly switch between ionization modes without the need for specialized tools. A safety relay switches off the high voltage supply (8 kV) when you remove the source from the mass spectrometer. A window at the front side of the ion source housing permits viewing the probe position during ESI operation and the addition of accessories.



Figure 3-4. OptaMax NG API source (HESI mode)

#### **Ion Source Mount**

The ion source mount on the front side of the mass spectrometer allows interchanging HESI, APCI, APPI, and calibration probes without using tools. The mount has high-voltage electrical connections for the electrospray needle (ESI and HESI) and for the vaporizer and corona discharge needle (APCI). See Figure 3-5. When you remove the ion source, a high-voltage safety interlock switches the statuses of various instrument components:

- ESI and HESI spray voltage (or APCI corona discharge voltage) is switched off.
- All API source and lens voltages, including the ion transfer tube offset voltage are switched off.
- Gases are switched off.
- The instrument is switched to standby condition if it was on before.



Figure 3-5. Ion source mount (Orbitrap Exploris 480 MS)

No.	Description	No.	Description
1	Connector for heater power and signal connections (readbacks and safety interlock)	2	Sheath gas outlet
3	Ion Source Housing Guide Pins	4	Ion source drain
5	Sweep Cone	6	Auxiliary gas outlet
7	High Voltage (8 kV) socket		

#### **Solvent Drainage**

The OptaMax NG API source can accommodate high flow rates. Therefore, you must collect the waste solvent in a manner that does not build up pressure in the source. The Orbitrap Exploris Series MS has a built-in drain. It routes the solvent waste from the API source (see Figure 3-5) to the solvent waste container that is connected to the source drain port at the left side of the instrument (see Figure 3-8 on page 3-17). For information about the solvent waste connection, see "Connecting the Source Housing Drain to the Solvent Waste Container" on page 5-20.

#### **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). Orbitrap Exploris Series instruments have two types of ion source interfaces:

- The ion source interface with an S-lens is used with the Orbitrap Exploris 120, Orbitrap Exploris 240, and Orbitrap Exploris MX MSs.
- The ion source interface with an ion funnel is used with the Orbitrap Exploris 480 MS.

See also page 3-26 for a complete overview of the ion optics.

#### Ion Source Interface with an S-Lens

For the Orbitrap Exploris 120, Orbitrap Exploris 240, and Orbitrap Exploris MX MSs, the API source interface includes a sweep cone, an ion transfer tube, two cartridge heaters, a heater block, a sensor, a vent prevent ball, and the S-lens (Figure 3-6).



Figure 3-6. API source interface with S-lens

No.	Description	No.	Description
1	Sweep cone	2	Vent prevent ball
3	Ion transfer tube	4	IC unit
5	S-lens	6	Heater block
7	Spray cone (directly behind the sweep cone)		

The sweep cone is a metal cone over the ion transfer tube. The sweep cone channels the sweep gas toward the entrance of the ion transfer tube, acts as a physical barrier that protects the entrance of the ion transfer tube, and increases source robustness. The net result is a significant increase in the number of samples to analyze without a loss of signal intensity.

**Tip** In addition, keeping the ion transfer tube entrance as clean as possible reduces the need for frequent maintenance. Install the sweep cone to improve ruggedness when you analyze complex matrices such as plasma or nonvolatile salt buffers. Remove the sweep cone before you perform NSI experiments.

The ion transfer tube assists in desolvating ions that are produced by the API probe. The tube is an elongated cylindrical tube made of metal. The heater block contains two heater cartridges, surrounds the ion transfer tube, and heats the tube to temperatures up to 400 °C (752 °F). A thermocouple measures the temperature of the heater block. Typical temperatures of the ion transfer tube are 320 °C (608 °F) for HESI and 275 °C (527 °F) for APCI, but these temperatures vary with the flow rate and the mobile phase composition. A decreasing pressure gradient draws ions into the ion transfer tube in the vacuum manifold. When you remove the ion transfer tube (after it has cooled to room temperature), the vent prevent ball drops into place to stop air from entering the vacuum manifold. Therefore, you can remove the ion transfer tube for cleaning or replacement without venting the system. See page 8-28 for details.

Ions from the ion transfer tube enter the S-lens. The S-lens is an ion transmission device that consists of progressively-spaced, stainless-steel electrodes. The MS applies an RF voltage to the electrodes of the S-lens to focus the ions toward the opening of the IC unit. Adjacent electrodes have voltages of opposite phase. As the RF amplitude increases, ions of progressively higher mass-to-charge ratios pass through to the IC source heater interface. When you tune the mass spectrometer, adjust the S-lens RF to maximize sensitivity. During the tune procedure, the mass spectrometer determines the mass-dependent RF amplitudes for optimum transmission of ions through the S-lens.

Ions from the S-lens pass through the IC unit and move toward the injection filter. The S-lens and the IC unit<sup>1</sup> act as a vacuum baffles between the higher-pressure ion source interface region and the lower-pressure ion optics region of the vacuum manifold. The S-lens and the IC unit mount to the ion source interface cage.

<sup>&</sup>lt;sup>1</sup> See also page 3-28 for information about the IC source.

#### Ion Source Interface with an Ion Funnel

For the Orbitrap Exploris 480 MS, the API source interface includes a sweep cone, an ion transfer tube, two cartridge heaters, a heater block, a sensor, a vent prevent ball, and the ion funnel (Figure 3-7).

The sweep cone is a metal cone over the ion transfer tube. The sweep cone channels the sweep gas toward the entrance of the ion transfer tube, acts as a physical barrier that protects the entrance of the ion transfer tube, and increases source robustness. The net result is a significant increase in the number of samples to analyze without a loss of signal intensity.

**Tip** In addition, keeping the ion transfer tube entrance as clean as possible reduces the need for frequent maintenance. Install the sweep cone to improve ruggedness when you analyze complex matrices such as plasma or nonvolatile salt buffers. Remove the sweep cone before you perform NSI experiments.



Figure 3-7. API source interface with ion funnel

No.	Description	No.	Description
1	Sweep cone	2	Vent prevent ball
3	Ion transfer tube	4	IC unit
5	Ion funnel	6	Heater block
7	Spray cone (directly behind the sweep cone)		

The ion transfer tube is a metal tube that has a rectangular orifice. It assists in desolvating ions that are produced by the API spray insert while transferring them into the vacuum system.

The heater block contains two heater cartridges, surrounds the ion transfer tube, and heats the tube to temperatures up to 400 °C (752 °F). A thermocouple measures the temperature of the heater block. Typical temperatures of the ion transfer tube are 320 °C (608 °F) for HESI and 275 °C (527 °F) for APCI, but these temperatures vary with the flow rate and the mobile phase composition. A decreasing pressure gradient draws ions into the ion transfer tube in the vacuum manifold. When you remove the ion transfer tube (after it has cooled to room temperature), the vent prevent ball drops into place to stop air from entering the vacuum manifold. Therefore, you can remove the ion transfer tube for cleaning or replacement without venting the system. See page 8-28 for details.

Ions from the ion transfer tube pass through the ion funnel and then the IC unit (Figure 3-15 on page 3-26). The ion funnel is an ion transmission device that consists of equally spaced, stainless-steel electrodes. The mass spectrometer applies an RF voltage to the electrodes, and adjacent electrodes have voltages of opposite phase. As the RF amplitude increases, ions of progressively higher mass-to-charge ratios pass through to the IC unit and move toward the injection filter. The IC unit<sup>1</sup> acts as a vacuum baffle between the higher-pressure API source interface region and the lower-pressure ion optics region of the vacuum manifold. The ion funnel and the IC unit mount to the API source interface cage.

<sup>&</sup>lt;sup>1</sup> See also page 3-28 for information about the IC source.
# **Left Instrument Side**

The forevacuum ports, the source drain port, and the gas inlets are at the left side of the instrument. Figure 3-8 shows the left side connections of an Orbitrap Exploris MX MS.



Figure 3-8. Connections at the left instrument side

No.	Description	No.	Description
1	Vacuum port for auxiliary forepump <sup>a</sup>	2	Vacuum port for source vacuum pump
3	Source drain port	4	Gas inlets: • Source & Vent (top) • C-Trap & HCD (bottom)

This port is not present in the Orbitrap Exploris 120, Orbitrap Exploris 240, and Orbitrap Exploris MX MSs.

## **Forevacuum Ports**

Connect the source vacuum pump to the large vacuum port (38 mm  $[1\frac{1}{2}$  in.] OD) at the left side of the instrument. Connect the auxiliary forepump of the Orbitrap Exploris 480 MS to the small vacuum port (19 mm  $[\frac{3}{4}$  in.] OD). Corresponding sections of reinforced PVC tubing are shipped with the instrument. For detailed information about the vacuum system, see page 3-37.

## **Source Drain Port**

The mass spectrometer internally routes the solvent waste from the
bottom of the API source to the back drain/waste port at the left side of
the instrument. For information about the solvent waste connection, see
"Connecting the Source Housing Drain to the Solvent Waste
Container" on page 5-20.

#### **Gas Inlets**

Two gas inlet ports are at the bottom of the left side of the instrument. The port for source gas & vent gas (top) has a press-in fitting for a 6 mm hose. The port for C-Trap gas & HCD collision gas (bottom) has a Swagelok<sup>™</sup>-type fitting for 1/16 in. tubing. See "Gas Supply" on page 5-12 for instructions for connecting the nitrogen supply of the laboratory to the instrument.



Do not connect other gases than nitrogen to the Orbitrap Exploris Series MS! This might affect instrument performance. The maximum pressure for the gas inlet is 0.65 MPa (6.5 bar, 94 psi).

Use high-purity (HP, 99%) nitrogen for the API source gases (sheath gas, auxiliary gas, and sweep gas). The HP nitrogen is also used to vent the vacuum manifold with the vent valve if the system is shut down. The collision gas (trapping gas) of the C-Trap, the collision gas for the ion-routing multipole, and the reagent carrier gas of the IC source require ultra-high purity (UHP, 99.999%) nitrogen. The necessary gas pressure is  $0.6 \pm 0.05$  MPa ( $6 \pm 0.5$  bar,  $87 \pm 7$  psi).

#### Gas Supply for the API Source, IRM, and C-Trap

The gas flow from the top gas port is directed through a Teflon<sup>™</sup> hose to the Source PCB. On the Source PCB, a valve terminal divides the nitrogen flow into three streams (sheath gas, auxiliary gas, and sweep gas) to the API source. Also, a T-piece directs part of the nitrogen flow into the vent valve (see page 3-39 for further information). When the instrument switches off, the vent valve opens and the nitrogen is led through stainless steel tubing to the vacuum manifold. The nitrogen gas flow ensures a clean and controlled venting of the instrument.

The gas flow from the bottom gas port is directed through 1/16 in. tubing to a pressure regulator, which keeps the gas pressure to the C-Trap and the ion-routing multipole constant. An electronic pressure regulator sets the nitrogen pressure according to the operating mode of the instrument and the chosen user setting. From the electronic regulator, a small part of the gas is led as collision gas to the ion-routing multipole behind the C-Trap. The larger part of the nitrogen stream is diverted into the source vacuum.

Left Instrument Side



Figure 3-9. Schematic of the internal gas supplies in MS/IC system

No.	Description	No.	Description
1	IC source	2	Calibrant distribution assembly (with fluoranthene oven and heated split)
3	API source	4	Source PCB
5	Source gas & vent gas inlet (top)	6	C-Trap & HCD gas inlet (bottom)
7	Regulator	8	Electronic pressure regulator
9	Ion-routing multipole	10	C-Trap
11	Vent valve		

#### **Gas Supply for the IC Source**

Two gas streams are directed from the input line of the HCD collision gas (UHP nitrogen) to the calibrant distribution assembly next to the API source. One gas stream provides a constant vapor pressure of the calibrant species to the IC source. The other gas stream provides the correct gas pressure to the discharge region to allow for a stable discharge. See Figure 3-9.

**Tip** When the IC source is in operation, the consumption of UHP nitrogen gas (as used for the C-Trap and the ion-routing multipole) increases significantly: 30 sccm ( $\approx 0.03 \ln/\min$ ) base flow plus a make up flow of up to 35 sccm ( $\approx 0.04 \ln/\min$ ).

# **Right Instrument Side**

Figure 3-10 shows the right side of the instrument. Visible are the control panel, power column, ventilation slots, and the accessories cabinet.



Figure 3-10. Right side of instrument (partial view)

No.	Description	No.	Description
1	Accessories Cabinet	2	Power Column
3	Control Panel	4	Ventilation Slots

## **Control Panel**



Figure 3-11. Control panel

No.	Description	No.	Description
1	Ethernet connector	2	D-sub port for forepump control
3	Peripheral control connectors	4	System reset

The *reset button* is located on the control panel. When you press the reset button, the instrument software is reloaded from the data system. See "Resetting the System" on page 6-13 for information on resetting the mass spectrometer.

**Tip** Use the reset button only if the instrument does not respond to the control program on the data system computer or if you must restart the instrument without switching off the electronics service switch.

Use the Ethernet port to connect the mass spectrometer to the data system computer.

Use the D-sub port to connect the remote control cable that is used for switching the forepump with a contact closure (relay output) signal. See "Forepumps" on page 3-38.

The Orbitrap Exploris Series MS has identical connectors (Peripheral A, Peripheral B) to communicate with two peripherals (LCs, for example) by digital and analog signals.

Port	Description			
±Digital in	+ (positive, pin 1) and – (negative, pin 2)			
	Based on the configuration, the mass spectrometer starts the data acquisition when it receives a digital contact closure signal from an external device.			
Digital out 1 Digital out 2 (interchangeable)	The mass spectrometer transmits the ready status through contact closure to an external receiving device.			
	The mass spectrometer transmits a programmable contact closure output signal to the inputs of an external receiving device (a fraction collector, for example).			
Analog In ±10 V	+ (positive, pin 7) and – (negative, pin 8) The mass spectrometer can record an analog signal between –10 V and +10 V from an external device with the mass spectrometer data.			

Table 3-6.	Peripheral	control	connectors
	i criprici ai	0011101	00111001013

Refer to the Help for information about setting up the communication with external devices.

The contact closure signals are transmitted through a trigger cable that connects the respective port to the external device. Suitable plug connectors for the peripheral control connection are provided with the Installation Kit. See "User I/O Connections" on page 5-28 for specifications of the peripheral control input connection ports.

#### **Power Column**

The power column at the right side of the instrument provides switches and connections that concern connections for power supply for the instrument and peripherals. See Figure 3-12.



Figure 3-12. Power column

No.	Description	No.	Decription
1	Holders for power supplies of syringe pump and switching valve	2	Mains supply connector
3	Power supply for syringe pump and switching valves (Total maximum current 3 A)	4	Main Power switch
5	Electronics service switch		

The *electronics service switch* is located at the top position of the power column. In the Service Only position, the switch removes power from most components of the mass spectrometer. In the Operating Mode position, power is supplied to all components of the mass spectrometer. Only qualified service personnel should operate the switch.

The *main power circuit breaker switch* (labeled Main Power) is located in the middle of the power column. In the OFF (O) position, the circuit breaker removes all power from the mass spectrometer, including the turbomolecular pump. It switches off the forepump by the remote control cable. In the ON (|) position, power is supplied to the mass spectrometer. In the standard operational mode, the circuit breaker is kept in the ON (|) position.

**Tip** Power is to remain on. The mass spectrometer should remain on and pumping continuously for optimum performance.

Both switches contain circuit breakers that protect the electrical wiring of the instrument from an overloaded (overcurrent) condition when it is exposed to more electrical current than it is designed to handle. In case of a thermal overload they interrupt the power supply to the instrument. After cooling down (and removal of the overload), the circuit breakers close and both switches can be used again. If you cannot reset the instrument to the operating mode despite repeated tries, the circuit breaker inside the switch is blown. In this case, call a Thermo Fisher Scientific field service engineer to replace it.

Use the four power outlets below the main power circuit breaker to supply electric power for low power devices of the LC/MS system (for example, a syringe pump or switching valves). These outlets are rated at 208–240 V AC, 50/60 Hz, 3 A total maximum. They are controlled by the main power circuit breaker switch and not by the electronics service switch.

Use separate wall outlets to supply electrical power for the forepump, the data system, and the devices of the LC/MS system if applicable.

The power connector for the mains supply is located below the four power outlets. Orbitrap Exploris Series instruments are designed to operate at a nominal voltage of 208–240 V AC, 50/60 Hz. See "Power Supply" on page 5-10 for details.

#### **Accessories Cabinet**

The accessories cabinet provides space for operating the syringe pump and the switching valves. The interior of the cabinet can be accessed by lifting the lid of the accessories cabinet. See Figure 3-13.



Figure 3-13. Accessories cabinet

Four USB ports allow the internal computer to communicate with other approved devices of the LC/MS system (for example, syringe pump). Do not connect any device to these ports other than dedicated Thermo Fisher Scientific devices.



Figure 3-14. USB ports

# Ion Optics

The ion optics focus the ions that are produced in the API source and transmit them to the C-Trap.

## Inlet Stack of the Orbitrap Exploris Series MSs with S-Lens

For the Orbitrap Exploris 120, Orbitrap Exploris 240 MS, and Orbitrap Exploris MX MSs, the inlet stack includes a heated ion transfer tube that assists in desolvating the ions. The tube guides the ions to an ion transmission device, the S-lens. The S-lens consists of progressively-spaced, stainless-steel electrodes to which an RF voltage is applied to transport and focus the ions to the Internal Calibrant Source. From there, the ions move toward the injection filter and the bent flatapole, which form the Advanced Active Transfer Tube Beam Guide (AABG).



Figure 3-15. Schematic of Orbitrap Exploris Series MSs with S-Lens

No.	Description	No.	Description
1	Transfer Tube	2	EASY-IC Internal Calibrant Source
3	Advanced Active Transfer Tube Beam Guide	4a	Advanced Quadrupole Technology (AQT) <sup>a</sup>
	(AABG)	4b	Transfer Quadrupole <sup>b</sup>
5	High Field Orbitrap Mass Analyzer	6	Ion-Routing Multipole
7	C-Trap	8	Independent Charge Detector
9	S-Lens	10	OptaMax NG Electrospray Ion Source

<sup>a</sup> Orbitrap Exploris 120, Orbitrap Exploris 240 MSs

<sup>b</sup> Orbitrap Exploris MX MS

## Inlet Stack of the Orbitrap Exploris Series MS with Ion Funnel

For the Orbitrap Exploris 480 MS, the inlet stack includes a heated high-capacity ion transfer tube—with a rectangular orifice—that assists in desolvating the ions. The tube guides the ions to an ion transmission device, the ion funnel. This device consists of a stack of electrodes to which an RF voltage is applied to transport and focus the ions to the Internal Calibrant Source. From there, the ions move toward the injection filter and the bent flatapole, which form the Advanced Active Transfer Tube Beam Guide (AABG). The ion funnel is controlled by the Funnel RF Driver, and its vacuum chamber is evacuated by the source vacuum pump.



Figure 3-16. Schematic of the Orbitrap Exploris 480 MS

No.	Description	No.	Description
1	High Capacity Transfer Tube	2	EASY-IC Internal Calibrant Source
3	Advanced Active Transfer Tube Beam Guide (AABG)	4	Advanced Quadrupole Technology (AQT)
5	Ultra-High Field Orbitrap Mass Analyzer	6	Ion-Routing Multipole
7	C-Trap	8	Independent Charge Detector
9	Electrodynamic Ion Funnel	10	OptaMax NG Electrospray Ion Source

## **Internal Calibrant Discharge Source**

The Internal Calibrant discharge source is installed in the IC source heater interface, which is located in the API source interface just after the S-lens or the ion funnel. Figure 3-17 shows the Internal Calibrant discharge source of an Orbitrap Exploris 480 MS.



Figure 3-17. Internal Calibrant discharge source and ion funnel (rear view)

The Internal Calibrant discharge source delivers a regulated number of calibrant ions into the much larger population of analyte ions. The internal calibrant ions are used as a lock mass (m/z) that significantly improves the mass-to-charge ratio (m/z) assignment accuracy to less than 1 ppm (up to m/z 1500) in every Fourier transform (FT) mass spectrum.

The instrument software uses the precisely known mass-to-charge ratio of the calibration mass peak to provide real-time fine adjustment of the instrument's mass-to-charge ratio calibration, enabling a correction for otherwise uncompensated errors that occur due to temperature changes and scan-to-scan variations in the total charge of the population of ions analyzed.

#### **Internal Calibrant Introduction**

The Internal Calibrant discharge source has its own dedicated continuous introduction system that delivers a highly stable flow of fluoranthene as calibrant. The calibrant distribution assembly receives an initial charge of fluoranthene during the installation. You can expect this charge to last at least one year. Only a Thermo Fisher Scientific field service engineer can replace the calibrant when it is consumed. A glow discharge electrode stably produces a very intense current of fluoranthene radical anions and a moderate current of fluoranthene radical cations. When you switch on the IC, it uses the radical anions (negative polarity) and cations (positive polarity) of fluoranthene as the internal calibration lock mass.

#### **Calibrant Distribution Assembly**

The calibrant distribution assembly connects through the vacuum manifold to the terminals of the IC source heater interface to deliver the calibrant (fluoranthene) to the calibrant ion source for ionization and further IC use. The assembly consists of:

- a pressure reducer with open split into vacuum and gas restrictors to provide a very low, constant flow of UHP nitrogen into the oven;
- the oven containing fluoranthene;
- a heated split where the make-up gas is mixed in, coming from the Porter pressure regulating unit through a gas restrictor;
- an interface to the IC source heater interface in the vacuum of the MS.

See page 3-19 for information about the gas supply for the IC source.



#### **IC Source Heater Interface**

Figure 3-18. Close-up view of the calibrant ion source in the IC source heater interface

The IC source heater interface is located in the API source interface region between the ion funnel and the injection filter. It consists of a

	mounting assembly that includes the calibrant ion source heater, a gas conduit, a high voltage contact, and the calibrant ion source.
	Figure 3-18 shows the IC source heater interface with a close-up view of the front of the calibrant ion source. The calibrant ion source contains the internal ion volume where reagent ion species are created, the discharge cathode, the anode, and a ceramic insulator.
	The calibrant ion source is a consumable part. For replacement instructions, see page 8-16.
Bent Flatapole	
	The bent flatapole always acts as an ion transmission device. It guides the ions through an arc from the injection filter to the quadrupole or transfer quadrupole and removes the neutral gas jet and solvent droplets that pass through the ion funnel and the injection filter. The neutral particles cannot follow the bent path of the flatapole.
	An RF voltage with a common-mode DC offset enables an efficient ion transport and the separation from neutrals. An additional axial DC gradient is applied to the bent flatapole to accommodate a fast ion transport.
Quadrupole Mass Filter	
	The Orbitrap Exploris 120, Orbitrap Exploris 240, and Orbitrap
	segmented hyperbolic quadrupole is used to provide the best transmission efficiency and rectangular transmission window shapes. The entrance segment is driven by RF voltage only, so that ions entering the quadrupole stay well focused before entering the middle section, the resolving quadrupole. Similarly, the exit section of the quadrupole also minimizes the fringe field regions and allows precise focusing. This is important for proper transfer of the ions to the C-Trap.
	<ul> <li>Exploits 480 Miss use advanced quadrupole technology (AQ1). A segmented hyperbolic quadrupole is used to provide the best transmission efficiency and rectangular transmission window shapes. The entrance segment is driven by RF voltage only, so that ions entering the quadrupole stay well focused before entering the middle section, the resolving quadrupole. Similarly, the exit section of the quadrupole also minimizes the fringe field regions and allows precise focusing. This is important for proper transfer of the ions to the C-Trap.</li> <li>In a quadrupole rod assembly, rods opposite each other in the array are connected electrically. Thus, the four rods can be considered as two pairs of two rods each. RF voltages and resolving DC voltages are applied to the rods and these voltages are adjusted for each 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 3-19.</li> </ul>

In Figure 3-20, the solid line represents the combined RF voltage and resolving DC voltage applied to one rod pair, and the dashed line represents the combined RF voltage and resolving DC voltage applied to the other rod pair. The RF-to-DC-voltage ratios and their values determine the range of mass-to-charge ratios to be transmitted through the quadrupole mass filter.

In the mass spectrometer, the rods of the quadrupole are supplied with a variable ratio of RF voltage and resolving DC voltage (Figure 3-20). For each injection, controlled by the split lens, the quad RF amplitude and resolving DC voltage are set to fixed values. Under these conditions, only ions of a certain range of m/z ratios are maintained within bounded oscillations as their velocity carries them through the mass filter. At the same time, all other ions undergo unbounded oscillations. These ions strike one of the rod surfaces, become neutralized, and are pumped away.



**Figure 3-19.** Polarity of the RF voltages and resolving DC voltages applied to the rods of the quadrupole mass filter





The quadrupole offset voltage is a DC potential applied to the quadrupole rods in addition to the filtering DC voltage. The offset voltage applied to the two rod pairs of the assembly is equal in amplitude and equal in sign. The quadrupole offset voltage accelerates or decelerates ions and, therefore, sets the translational kinetic energy of the ions as they pass the quadrupole rod assembly.

### **Independent Charge Detector**

The independent charge detector (ICD) is positioned between the quadrupole and the C-Trap. It is used to increase the fidelity of the Automatic Gain Control (AGC) in certain operation modes. The assembly includes a split lens, which is used to start and stop the injection of ions into the C-Trap. A precise determination of the ion beam intensity and a fast switching of the ion beam are needed for the Automatic Gain Control (AGC) of the Orbitrap mass analyzer. The assembly also includes a short transport RF multipole, which is the interface between the ICD and the C-Trap.

# **Curved Linear Trap**

The MS always passes the ions through the gas-filled curved linear trap (C-Trap) before trapping them in the ion-routing multipole. See Figure 3-15 on page 3-26. The MS then passes the ions back to the C-Trap before injecting them into the Orbitrap mass analyzer.

The ions that enter the C-Trap lose their kinetic energy by colliding with the nitrogen collision gas, which dissipates their kinetic energy and cools them down to the center axis of the C-Trap.

Voltages on the end apertures of the C-Trap (entrance and exit apertures) are controlled to provide or avoid a potential well along its axis. These voltages may be later ramped up to squeeze ions into a shorter thread along this axis.

# **Ion-Routing Multipole**

The ion-routing multipole (IRM) consists of a straight multipole that is mounted inside an enclosed assembly, which is connected in direct line-of-sight to the C-Trap. The MS supplies the IRM with the nitrogen collision gas to increase the multipole's gas pressure. The C-Trap is directly attached to the IRM, so part of the collision gas also flows into the C-Trap. See "Gas Supply for the API Source, IRM, and C-Trap" on page 3-18 for details.

For Full Scan operation, the IRM is used to cool and trap the ions. A potential gradient is used to effectively transport the ions back towards the C-Trap.

For HCD (Higher Energy Collisional Dissociation)<sup>1</sup>, ions pass through the C-Trap into the IRM. The offset voltage between the C-Trap and the IRM accelerates the precursor ions into the gas-filled IRM leading to fragmentation. The MS applies a potential gradient to the IRM to provide fast extraction of ions, such that it returns ions at a reliable rate. The spectra of the fragments generated in the IRM and detected in the Orbitrap analyzer are comparable to the typical fragmentations patterns obtained on triple-quadrupole instruments.

<sup>&</sup>lt;sup>1</sup> Not available for the Orbitrap Exploris MX MS.

# **Orbitrap Analyzer**

The heart of the Orbitrap<sup>™</sup> analyzer is an axially-symmetrical mass analyzer. It consists of a spindle-shape central electrode surrounded by an outer electrode that is split into bell-shaped halves. See Figure 3-21. The Orbitrap analyzer employs electric fields to capture and confine ions. The specifications for the Orbitrap analyzer in the Orbitrap Exploris 480 MS are more stringent than those for an Orbitrap analyzer in one of the other instruments.







## **Extraction of Ion Packets**

For ion extraction, the RF voltage on the rods of the C-Trap is ramped off and extracting voltage pulses are applied to the electrodes, pushing ions orthogonally to the curved axis through a slot in the inner electrode. Because of the initial curvature of the C-Trap, including the Z-Lens, and the subsequent lenses, the ion beam converges on the entrance into the Orbitrap analyzer. The lenses that follow the C-Trap (Z-lens) also act as differential pumping slots and cause spatial focusing of the ion beam into the entrance of the Orbitrap analyzer. In the Z-Lens, ions are electrostatically deflected away from the gas jet, thereby eliminating gas carryover into the Orbitrap analyzer.

Owing to the fast pulsing of ions from the C-Trap, ions of each mass-to-charge ratio arrive at the entrance of the Orbitrap analyzer as short packets that are only a few millimeters long. For each mass-to-charge population, this corresponds to a spread of flight times of only a few hundred nanoseconds for mass-to-charge ratios of a few hundred Daltons per charge. Such durations are considerably shorter than a half-period of axial ion oscillation in the Orbitrap analyzer. Because ions are injected into the Orbitrap analyzer at a position offset from its equator (see Figure 3-22), these packets start coherent axial oscillations without the need for any additional excitation cycle. The evolution of an ion packet during an increase of the electric field is shown schematically in Figure 3-22. When the injected ions approach the opposite half of the outer electrode for the first time, the increased electric field (owing to the change of the voltage on the central electrode) contracts the radius of the ion cloud by a few percent. The applied voltages are adjusted to prevent collision of the ions with the electrode. A further increase of the field continues to squeeze the trajectory closer to the axis, meanwhile allowing for newly arriving ions (normally, with higher m/z) to enter the Orbitrap analyzer as well. After ions of all m/z have entered the Orbitrap analyzer and moved far enough from the outer electrode, the voltage on the central electrode is kept constant and image current detection takes place.



r = radial position; z = axial position

**Figure 3-22.** Principle of electrodynamic squeezing of ions in the Orbitrap analyzer as the field strength is increased

No.	Description	No	Description
1	Deflector electrode	2	Central electrode
3	Outer electrode		

## **Measuring Principle**

In the mass analyzer shown in Figure 3-21 on page 3-34, stable ion trajectories combine rotation around an axial central electrode with oscillations along it. The Orbitrap analyzer's electrodes are shaped such that the ions experience a quadro-logarithmic potential, for which their axial oscillations are harmonic. The frequency  $\omega$  of these harmonic oscillations along the z-axis depends only on the ion's mass-to-charge ratio m/z and the instrumental constant k:

$$\omega = \sqrt{\frac{z}{m} \times k}$$

The split halves of the outer electrode of the Orbitrap analyzer detect the image current produced by the oscillating ions. By Fast Fourier Transformation (FFT) of the amplified image current, the instrument obtains the frequencies of these axial oscillations and thus, the mass-to-charge ratios of the ions.

# Ion Detection

During ion detection, the central electrode and the additional electrode (see Figure 3-22), which deflects the ions during the injection and compensates electric field imperfections during the measurement, are maintained at very stable voltages so that no mass drift can take place. The outer electrode is split in half at z=0, allowing the ion image current in the axial direction to be collected. The image current on each half of the outer electrode is differentially amplified and then undergoes analog-to-digital conversion before processing by the fast Fourier transform algorithm.







As mentioned above, stable ion trajectories in the Orbitrap analyzer combine axial oscillations along the z-axis with rotation around the central electrode and vibrations in the radial direction. (See Figure 3-21 on page 3-34.) For any given m/z, only the frequency of axial oscillations is completely independent of initial ion parameters, whereas rotational and radial frequencies exhibit strong dependence on initial radius and energy. Therefore, ions of the same mass-to-charge ratio continue to oscillate along z together, remaining in-phase for many thousands of oscillations.

In contrast to the axial oscillations, the frequencies of radial and rotational motion will vary for ions with slightly different initial parameters. This means that in the radial direction, ions dephase orders of magnitude faster than in the axial direction, and the process occurs in a period of only 50–100 oscillations. After this, the ion packet of a given m/z assumes the shape of a thin ring, with ions uniformly distributed along its circumference. See Figure 3-23. Because of this angular and radial smearing, radial and rotational frequencies cannot appear in the measured spectrum. Meanwhile, axial oscillations will persist, with axial thickness of the ion ring remaining small compared with the axial amplitude. Moving from one half of the outer electrode to the other, this ring will induce opposite currents on these halves, thus creating a signal to be detected by differential amplification.

# **Vacuum System**

The vacuum manifold encloses the ion source interface, the ion guides, the C-Trap, and the Orbitrap analyzer. The vacuum manifold consists of thick-walled aluminum chambers with machined flanges on the front, the sides, and the bottom, and various electrical feedthroughs and gas inlets. The vacuum manifold is divided into seven chambers. The region inside the first chamber, called the S-lens region or funnel region, is evacuated by an external roughing pump (source vacuum pump). An internal six-stage turbomolecular pump (TMP) applies a vacuum of increasing quality along the other six regions, the sixth region being evacuated by the UHV stage of the TMP. Figure 3-24 shows a schematic overview of the vacuum system, Table 3-7 shows the vacuum regions of the mass spectrometer.



Figure 3-24. Schematic of vacuum system in Orbitrap Exploris Series MS

	Table 3-7.	Vacuum	regions	overview
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Region in instrument	Vacuum [mbar]	Gauge type	applied by
Ion source housing	1E+03		Atmosphere
S-lens region <sup>a</sup>	$2^{\mathrm{b}}$	Pirani	Source we are the second
Funnel region <sup>c</sup>	3.5 <sup>b</sup>	-	Source vacuum pump
Injection filter <sup>c</sup>			TMP IS5
Bent flatapole		Pirani <sup>c</sup>	TMP IS4
Quadrupole / transfer quadrupole	4E-05	-	TMP HV
Z-lens			TMP IS2
Region between Z-lens and Orbitrap analyzer		Cold cathode	TMP IS1
Orbitrap analyzer	< 8E-10	-	TMP UHV
Ion-routing multipole	1.1E-2	Pirani	Collision gas

<sup>a</sup> Orbitrap Exploris 120, Orbitrap Exploris 240, and Orbitrap Exploris MX MS

<sup>b</sup> Depends on the temperature of the heated tube.

<sup>c</sup> Orbitrap Exploris 480 MS

	In the Orbitrap Exploris 480 MS, four vacuum gauges monitor the vacuum. In the other Orbitrap Exploris Series instruments, three gauges monitor the vacuum:
	• Orbitrap Exploris 480 MS: The vacuum in the funnel region is monitored by an Active Pirani gauge that is connected to the forevacuum line.
	Orbitrap Exploris 120, Orbitrap Exploris 240, Orbitrap Exploris MX MS: The vacuum in the S-lens region is monitored by an Active Pirani gauge.
	• Orbitrap Exploris 480 MS: The vacuum in the injection filter region is monitored by an Active Pirani gauge.
	This gauge is absent in the other Orbitrap Exploris Series instruments. In the Tune application, the vacuum in the TMP IS5 region (or inject filter region) shows as 0 mbar.
	• The vacuum in the ion-routing multipole is monitored by an Active Pirani gauge.
	• The vacuum in the Orbitrap analyzer chamber is monitored by a Cold Cathode Gauge. This gauge is directly mounted to the turbomolecular pump.
Forepumps	
	The Orbitrap Exploris 480 MS is shipped with a high-throughput source vacuum pump and a low-throughput auxiliary forepump:
	<ul> <li>The single-stage rotary vane pump is used as source vacuum pump. It evacuates the funnel region of the vacuum manifold. The pump has a nominal pumping speed of ≥110 m<sup>3</sup>/h.</li> </ul>
	• The two-stage rotary vane pump as auxiliary forepump supplies the forevacuum for the TMP. The pump has a nominal pumping speed of approximately 9 m <sup>3</sup> /h at 50 Hz / 10.5 m <sup>3</sup> at 60 Hz.
	For all other Orbitrap Exploris Series MSs, a single-stage rotary vane pump is used as forepump. It establishes the vacuum that is necessary for the proper operation of the TMP. The pump also evacuates the S-lens region of the vacuum manifold. The pump has a nominal pumping speed of about 60 m <sup>3</sup> /h.
	All forepumps come with separate noise reduction covers. The pumps are placed on drip pans with wheels or sliders below the workbench.
	<b>Tip</b> Thermo Fisher Scientific offers dry pumps as alternative to the standard forepumps. See page 5-8 for details.

The forepumps are switched on and off by a cable or a Y-cable<sup>1</sup> that is plugged into the D-sub port on the control panel at the right side of the MS. The power supply cords of the forepumps are plugged into separate wall outlets. The pumps automatically shut down when the communication with the mass spectrometer stops.

See page 5-6 for detailed information about connecting the forepumps to the MS and the laboratory infrastructure. For a detailed description of the forepumps and for instructions on user maintenance, refer to the handbooks of the manufacturer. See also "Maintenance of the Forepumps" on page 8-10.

### **Turbomolecular Pump**

A six-stage turbomolecular pump (TMP) provides the high vacuum for the mass spectrometer. The air cooled TMP is attached to the bottom of the vacuum manifold. A pump controller supplies power to the TMP and controls it. The controller sends status information of the TMP (such as temperature or rotational speed) to the MS and the data system. The main power circuit breaker switch turns off the TMP. The electronics service switch has no effect on the pumps.

For a detailed description of the TMP and for instructions on user maintenance, refer to the handbook for the pump. See also "Maintenance of the Turbomolecular Pump" on page 8-12.

The vent valve is a solenoid-operated valve that allows the vacuum manifold to be vented. The vent valve is closed when the solenoid is energized.

The vacuum manifold is vented when external power is removed from the instrument. (Power is removed from the instrument by a power failure or by placing the main power circuit breaker in the Off (O) position.) After the external power is removed, power is provided to the vent valve until the rotational speed of the TMP is reduced sufficiently to allow controlled venting of the instrument. If external power is not restored to the instrument in this time, 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 with nitrogen. See Figure 3-24 on page 3-37. The vent valve closes after power is restored to the instrument.

Vent Valve

<sup>&</sup>lt;sup>1</sup> In case of an Orbitrap Exploris 480 MS.

## System Bake-out

After the system has been open to the atmosphere (for example, during maintenance work or a power outage), the vacuum deteriorates due to contaminations of the inner parts of the vacuum system caused by moisture. These contaminations must be removed by heating the vacuum system: a system bake-out. See "Baking Out the System" on page 8-12 for instructions on performing a manual system bake-out.

Several heating elements inside the vacuum chamber provide the high temperatures that are necessary to perform a system bake-out.

# **Electronic Assemblies**

The electronic assemblies that control the operation of the mass spectrometer are distributed among various printed circuit boards (PCBs) and other modules, in the embedded computer, and on or around the vacuum manifold of the mass spectrometer. Dedicated electronic assemblies control the operation of the components of the Internal Calibration source such as heaters and pressure regulators. You cannot service the electronic assemblies.

**Tip** If you need assistance, contact your local Thermo Fisher Scientific field service engineer. Before you call a service engineer, try to find the defect by means of errors indicated in the Tune application. A precise description of the defect will ease the repair and reduce the costs. Running the appropriate diagnostics can provide further insights.

# **Cooling Fans**

Several fans, including those in the power supply subassemblies, provide internal cooling for the Orbitrap Exploris Series mass spectrometer. Cooling air enters through the three main air intake fans on three sides of the MS. Exhaust air leaves the instrument from the ventilation slots at the rear side and the top side.

The only user-serviceable part are the air filters in front of the air intake fans. For the recommended maintenance schedule, see "Maintenance of the Fan Filters" on page 8-14.

In addition to the fans described in this topic, various printed circuit boards are equipped with individual fans.

# **Additional Hardware**

In addition to connecting the Orbitrap Exploris Series mass spectrometer to one or two LC systems, you can use the instrument with a syringe pump or switching valves. With the accessories cabinet, the MS provides a place for the operation below a lid at the top right side of the instrument. See Figure 3-25.



Figure 3-25. Accessories cabinet with syringe pump

## **Syringe Pump**

You can connect the Orbitrap Exploris Series mass spectrometer to a syringe pump. The syringe pump delivers sample solution from the syringe into the API source. When the syringe pump is operating, a motor drives a pusher block that depresses the plunger of the syringe at a user selectable rate. Liquid flows out of the syringe needle and into the sample transfer line as the plunger is depressed. For instructions on setting up the syringe pump, see "Setting Up the Syringe" on page 5-24. A suitable syringe pump is shipped with the instrument.

The instrument software can control established syringe pumps by a USB interface in the accessories cabinet. See Figure 3-14 on page 3-25. The MS can supply electric power to the syringe pump with an outlet on the power column. See Figure 3-12 on page 3-23. Or, use a properly grounded wall outlet. "Setting Up the Inlet for Direct Infusion" on page 5-23 gives instructions on connecting the syringe pump to the MS.

You can set syringe pump parameters with the Tune application. Use the Tune application to switch on/off the syringe pump by an instrument method or manually. Refer to the Help for details.

## **Switching Valves**

You can connect the Orbitrap Exploris Series mass spectrometer up to two external switching valves. Suitable switching valves (Rheodyne<sup>™</sup> MX Series II<sup>™</sup>) are available from Thermo Fisher Scientific. The instrument software can control established switching valves by a USB interface in the accessories cabinet. See Figure 3-14 on page 3-25. The Universal Power Supply of the valve can be operated from inputs of 100–240 V AC, 50–60 Hz. The MS can provide electric power to the valves with an outlet on the power column. See Figure 3-12 on page 3-23. Or, use a properly grounded wall outlet.

You can configure (plumb) a switching valve as a loop injector for flow injection analysis or as a divert valve for direct infusion, high-flow infusion, or LC/MS experiments. Procedures for plumbing the valve in the loop injector or divert valve configuration are given in "Setting Up the Inlet for Direct Infusion" on page 5-23.

You can control the switching valves with the Tune application. Refer to the Help for instructions about operating the switching valves.

You can also use the switching valve button to divert the LC flow between the MS and waste when the valve is in the divert valve configuration. Or, you can switch between load mode and inject mode when the valve is in the loop injector configuration.

# Safety

This chapter contains information that is important for your own safety or the safety of others, and that prevents damage to the instrument, Read this chapter carefully before you install or operate the instrument and its accessories, or come into contact with it.

To comply with safety and warranty requirements, the instrument and accessories described in this manual are designed to be used only by properly trained personnel.

Any installation, adjustment and repair of this equipment must be carried out only by a certified Thermo Fisher Scientific service representative who is aware of the hazards involved.

To protect our operating personnel, we ask you to adhere to special precautions when you send back parts to the factory for exchange or repair. See "Returning Parts" on page 8-44.

#### Contents

- Safety Symbols and Signal Words in this Manual on page 4-2
- Safety Symbols on the Instrument on page 4-3
- Intended Use on page 4-5
- Electric Safety Precautions on page 4-8
- In Case of an Emergency on page 4-10
- Residual Hazards on page 4-12
- Personal Protective Equipment on page 4-14

# Safety Symbols and Signal Words in this Manual

Notices concerning the safety of the personnel operating the Orbitrap Exploris Series mass spectrometer appear different from the main flow of text:

	Always be aware of what to do with, and the effect of, safety information.
	Points out a hazardous situation that can lead to minor or medium injury if it is not avoided.
	Points out a hazardous situation that can lead to severe injury or death if it is not avoided.
<b>ADANGER</b>	Points out a hazardous situation that will lead to severe injury or death if it is not avoided.

## **Observing this Manual**

Keep this manual always near the instrument to have it available for quick reference.

Be sure to read and comply with all precautions described in this manual.

System configurations and specifications in this manual supersede all previous information received by the purchaser.

# Safety Symbols on the Instrument

Table 4-1 lists all safety labels on the instrument and their positions. See the indicated safety notices to prevent harm to the operator and to protect the instrument against damage. If present, read and follow the instructions on the labels.

**Table 4-1.**Safety labels on the instrument

#### Label Label description



This label is attached to the ion source mount at the front side of the instrument. It indicates the presence of high voltage at the ion source. See page 8-28 for details.



This label is attached to the ion source mount at the front side of the instrument. It indicates the presence of hot surfaces at the ion source mount. See page 8-36 for details.

This label is attached to the API probe. It indicates the presence of high voltage at the probe. See page 6-11 for details.

This label is attached to the ion source housing. It indicates the presence of hot surfaces at the ion source housing. See page 8-24 for details.



This label is attached to the ion source housing. It indicates that you must read the relevant user documentation before you use the ion source.





#### Label position





Labels of this type are attached to several places on the instrument that are designed for user interaction. They remind you to read the manual before you operate the instrument.

This label is attached to several places on the instrument that may be accessed by users. It indicates that only personnel that have received a special training may service the instrument. User maintenance is restricted to operations that are described in this manual.

Table 4-1.	Safety labels on the instrument, continued
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Label	Label description	Label position
	DANGER         Electrical hazard.         Will result in death or serious injury.         Disconnect power before removing cover.	This label is attached to several places on the instrument that may be accessed by users. It indicates that hazardous electric voltage is used in the instrument that can cause serious injury or even death. To make sure that the instrument is free from all electric current, always disconnect the power cord of the instrument before you remove the covers.
	WARNING Heavy object. Can cause back injury during transportation. See manual for instructions.	This label is attached to the rear side of the instrument. It indicates that, because of its weight, handling the instrument alone might cause muscle strain and back injury. See "Moving the Instrument" on page 5-4 for instructions.

### **Name Plate**

To identify the instrument correctly when you contact Thermo Fisher Scientific, always have the information from the name plate (also called rating plate) available. The name plate is attached below the power column at the right side of the instrument. It contains the serial number, which is important in any type of communication with Thermo Fisher Scientific. See Figure 4-1. Especially, the serial number is needed to get access to the SharePoint of the Bremen Technical Documentation group. See "Contacting Us" on page 1-5.



Figure 4-1. Name plate (example)

# **Intended Use**

Orbitrap Exploris Series mass spectrometers are stand-alone Orbitrap<sup>™</sup> instruments with an atmospheric pressure ionization (API) source for liquid chromatography (LC) mass spectrometry (MS) high-throughput applications.

▲ Observe the following usage guidelines when you operate the Orbitrap Exploris Series mass spectrometer:

- The instrument is designed to be placed on a bench in the laboratory. It is not designed for outdoor usage.
- The instrument is designed to be used exclusively with API sources and probes that are approved by Thermo Fisher Scientific.
- The instrument is designed for use as general lab equipment. It is not designed for use in diagnostic or medical therapeutic procedures.

If the instrument is used in a manner that is not specified by Thermo Fisher Scientific, the protection that is provided by the instrument could be impaired. Thermo Fisher Scientific assumes no responsibility and will not be liable for instrument damage and/or operator injury that might result from using the instrument with other API sources and probes.

#### Notice on the Susceptibility to Electromagnetic Transmissions

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

### **Qualification of the Personnel**



Personnel that install or operate the Orbitrap Exploris Series mass spectrometer must have the following qualifications:

- Electrical Connections
  The electrical installation must be made by qualified and skilled personnel (electrician) according to the appropriate regulations (for example, cable cross-sections, fuses, grounding connection).
  Refer to the *Orbitrap Exploris Series Pre-Installation Requirements Guide* for the specifications.
- Installation Only employees of Thermo Fisher Scientific or personnel who act on behalf of Thermo Fisher Scientific are allowed to install the Orbitrap Exploris Series mass spectrometer.

# General Operation The Orbitrap Exploris Series mass spectrometer is designed to be operated by qualified laboratory personnel. Before they start, all users must be instructed about the hazards that are presented by the instrument and by the used chemicals. The users must be advised to read the relevant Material Safety Data Sheets (MSDSs). Decommissioning Only employees of Thermo Fisher Scientific or personnel who act on behalf of Thermo Fisher Scientific are allowed to decommission the Orbitrap Exploris Series mass spectrometer. For information about decommissioning third-party components (for example, the forepump), refer to the manuals that came with these components.

The Orbitrap Exploris Series mass spectrometer is designed to be operated with these materials:

- Nitrogen gas: Used for the API sheath gas, the API auxiliary/sweep gas, the C-Trap trapping gas, the reagent carrier gas of the IC source, and the HCD collision gas
- Forepump oil: Used for the cooling, the lubrication, and the sealing of the forepump

Use only the forepump oil that is indicated on the name plate and pump. If other oils are used, the manufacturers reject all responsibility should any trouble occur. See page 9-3 for a specification of the forepump oil.

- Fluoranthene: Used as the calibrant species for the IC source
- Calibration compounds, samples

Polar or less polar chemical compounds—soluble in water or appropriate organic solvent. Compounds can have different molecular sizes. Compounds derive from environmental specimens of different origins. The origin can be from living or non-living matter. Examples are sugars (carbohydrates) from plant material, proteins or peptides from animal or human cell lines, synthetic polymers deriving from an organic synthesis. Small molecules can derive from a honey sample when screening for or quantifying pesticides or from an organic synthesis.

• Solvents, additives

> Typically, mixtures of water and organic solvents are applied. Organic solvents can be methanol, acetonitrile, or isopropanol. Also chloroform or dichloromethane are solvents applied when these are needed to solubilize the compounds of interest and to prepare them ready-to-use for the ion source interface.

## **Permitted Materials**

NOTICE

Common additives to the solvent mixtures are acids such as trifluoroacetic acid or formic acid (positive ion mode) or a base such as ammonium hydroxide (negative ion mode).

# **Electric Safety Precautions**

#### 

**High Voltage.** High voltages (up to 8 kV) that can cause an electric shock are used in the instrument. Observe these safety precautions when you operate or do maintenance on the instrument:

- The instrument is properly grounded in accordance with regulations when it is shipped. You do not need to make any changes to the electrical connections or to the instrument's chassis to ensure safe operation.
- There are no customer serviceable parts inside. Do not remove any housing or protective cover except it is permitted elsewhere in this manual. When you leave the system, make sure that all protective covers and doors are properly connected and closed, and that heated areas are separated and marked to protect unqualified personnel.
- Do not switch on the instrument if you suspect that it has incurred any kind of electrical damage. Instead, disconnect the power cords of the mass spectrometer and the forepump and contact a Thermo Fisher Scientific field service engineer for a product evaluation. Do not try to use the instrument until it has been evaluated. Electrical damage might have occurred if the system shows visible signs of damage, or has been transported under severe stress.
- Do not place any objects on top of the instrument—especially not containers with liquids—unless it is requested by the user documentation. Leaking liquids might get into contact with electronic components and cause a short circuit.

## Safety Protection provided by the Instrument

The Orbitrap Exploris Series system provides protection according to several isolation and safety standards for electronic instruments. See the "EU Declaration of Conformity" on page A-5 for information about the relevant standards.

#### **IEC Degree of Protection: IP20**

The Orbitrap Exploris Series system is resistant to solid foreign bodies from 12.5 mm in diameter (accidental finger contact), but it is not protected against the ingress of water.

### IEC Protection Class: I

The Orbitrap Exploris Series system has a protective ground connection and a basic insulation between accessible parts and the protective earth. A proper protective ground connection is compulsory.

#### IEC Overvoltage Category: II

The Orbitrap Exploris Series system has a plug and socket connector or a fixed connection supplied from the electrical system of a building.

#### **IEC Pollution Degree: 2**

The Orbitrap Exploris Series must be used in an environment where only non-conductive pollution occurs. Occasionally, temporary conductivity caused by condensation is to be expected.

# In Case of an Emergency

#### 

**Electric Current.** Electric shock hazard. Do not use the electronics service switch to shut down the instrument. See Figure 4-2. The electric components of the vacuum system will still be connected to the electric power supply and the pumps will remain running. Placing the main power circuit breaker switch on the power column in the Off (O) position may not be sufficient for safe work on the instrument.

#### \* To shut down the system in case of an emergency

1. Disconnect the power cord of the mass spectrometer to ensure that the instrument is free from all electric current. All power to the MS, including the internal vacuum pumps, is shut off. Also, all power to any devices that are supplied with power by the MS (for example, switching valves, syringe pump) is shut off.



Figure 4-2. Power column

No.	Description	No.	Description
1	Electronics service switch	2	Main Power switch
3	Power supply for syringe pump and switching valves	4	Mains supply connector
2. The forepumps are only switched off with the relay control cable. To disconnect a forepump from its electric power supply, unplug the power cord.

**Tip** The pumps shut down automatically when the communication with the mass spectrometer stops.

3. Switch off the computer with its On/Off switch.

# **Residual Hazards**

Users of the Orbitrap Exploris Series mass spectrometers must pay attention to these residual hazards. **High Voltage.** If you touch liquid that leaks from the probe sample inlet while the mass spectrometer is in operation, you might receive an electric shock. Do not tighten the probe sample inlet fitting to eliminate a liquid leak while the mass spectrometer is in operation. **Suffocation Hazard.** A significant amount of the nitrogen that is introduced into the API source can potentially escape into the laboratory atmosphere. Accumulation of nitrogen gas could displace sufficient oxygen to suffocate personnel in the laboratory. Make sure that the laboratory is well ventilated. Always operate the mass spectrometer and the API source with the attached drain tubing assembly that connects the source housing drain to a dedicated exhaust system. Local regulations may make a risk assessment for the workplace necessary. Electromagnetic Radiation. Parts of the forepump emit electromagnetic radiation. This radiation can interfere with the operation of cardiac pacemakers and implanted heart defibrillators, possibly causing death or serious injury. If you wear these devices, keep at least 30 cm away from the forepump. Hazardous Chemicals. Samples, solvents, and detergents might contain toxic, carcinogenic, mutagenic, or corrosive/irritant chemicals. Avoid exposure to potentially harmful materials. Always wear protective clothing, gloves, and safety glasses when you handle solvents or samples. Also contain waste streams and use proper ventilation. Refer to your supplier's Material Safety Data Sheet (MSDS) for proper handling of a particular compound. Hot Parts. The forepump in function is hot and some surfaces could reach a temperature higher than 80 °C (176 °F). Touching parts of the forepump might cause burns. Switch off the pump and let it cool down before any intervention. If you must work on a pump that is "still warm from operation," then always wear heat protective gloves.

# ▲ CAUTION Hot Parts. During operation of the mass spectrometer, the ion transfer tube and the sweep cone can reach temperatures up to 450 °C. This might cause severe burns upon touching or ignite combustible material. The external surface of the ion source housing can reach temperatures up to 100 °C. This is hot enough to cause skin burns. Do not touch the ion source housing when the mass spectrometer is in operation. Let the ion source cool down as described in this manual before you remove the ion source housing. Do not touch the ion source housing are removed the ion source housing. Keep combustible materials away from the ion source mount. Do not let the instrument stay unattended when the housing is not mounted to the source.



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

# **Personal Protective Equipment**

Appropriate safety clothing must be worn at all times while you operate the instrument, particularly when you handle hazardous material.

This manual can only give general suggestions for personal protective equipment (PPE), which protects the wearer from hazardous substances. Refer to the Material Safety Data Sheets (MSDSs) of the chemicals handled in your laboratory for advice on specific hazards or additional equipment.

#### **Eye Protection**

The type of eye protection required depends on the hazard. For most situations, safety glasses with side shields are adequate. Where there is a risk of splashing chemicals, goggles are necessary.

#### **Protective Clothing**

When the possibility of chemical contamination exists, protective clothing that resists physical and chemical hazards should be worn over street clothes. Lab coats are appropriate for minor chemical splashes and solids contamination, while plastic or rubber aprons are best for protection from corrosive or irritating liquids.

#### Gloves

For handling chemical compounds and organic solvents, Thermo Fisher Scientific recommends white nitrile clean room gloves from Fisher Scientific or Unity Lab Services.

For handling hot objects, gloves made of heat-resistant materials (for example, leather) should be available.

#### **Safety Boots and Shoes**

Safety boots and shoes which are penetration-resistant and feature protective toecaps can protect employees from falling objects, vehicles and other heavy loads, for example when moving the instrument.

# Installation

This chapter describes the conditions for an operating environment that will ensure continued high performance of your Orbitrap Exploris Series system.

To be sure that your laboratory is ready for the installation of the Orbitrap Exploris Series system, you have to meet all requirements that are specified in the *Orbitrap Exploris Series Pre-Installation Requirements Guide*. This guide also provides comprehensive information to assist in planning and preparing your lab site.

#### Contents

- Placing the Instrument on page 5-2
- Placing the Forepumps on page 5-6
- Laboratory Conditions on page 5-10
- Setting Up the Instrument Hardware and Adjusting the System Parameters on page 5-19
- Configuring the Ion Source on page 5-20
- Connecting Frequently Used Devices on page 5-23
- Obtaining the Calibration Solution on page 5-30

# **Placing the Instrument**

This section provides information that helps you positioning the instrument in the laboratory.

#### **Instrument Dimensions**

The body of the Orbitrap Exploris Series mass spectrometer has maximum dimensions of h 703 mm (27<sup>11</sup>/<sub>16</sub> in.), w 534 mm (21 in.), l 763 mm (30<sup>1</sup>/<sub>16</sub> in.). Figure 5-1 shows a schematic view of the instrument with important instrument dimensions.



Figure 5-1. Dimensions of MS

#### Workbench for Instrument

The Orbitrap Exploris Series MS is designed to be placed on top of a workbench with its rear panel against a wall. To set up a typical LC/MS system, Thermo Fisher Scientific recommends that you have a minimum of two workbenches. Table 5-1 lists the recommended minimum surface dimensions for each workbench.

**Table 5-1.**Minimum workbench surface dimensions

Equipment	Surface
Data system	$120 \times 100 \text{ cm} (47\frac{1}{4} \times 39\frac{3}{8} \text{ in.})$
LC/MS system	$150 \times 100 \text{ cm} (59^{1}/_{16} \times 39^{3}/_{8} \text{ in.})$

The workbench for the LC/MS system must be capable of supporting the weight of the mass spectrometer (about 120 kg) plus the weight of any option (liquid chromatograph, for example) and stand in a secure and level position.

▲ Only workbenches with four legs provide sufficient stability for the mass spectrometer. The workbench top must be dry and clean (free of grease). Thermo Fisher Scientific recommends that you use a workbench with a skidproof top.

Follow these clearance guidelines for the workbenches:

- Place the data system workbench and the LC/MS workbench adjacent to each other to prevent strain on the interconnecting Ethernet communications cables.
- Make sure that you have the following minimum clearances:
  - 900 mm (35½ in.) between the top of the system and any shelves above it.
  - 400 mm (16 in.) between the left side or the right side of the instrument and any other components.

Spacers at the rear side of the instrument provide sufficient space for airflow.

To allow shutting off the mass spectrometer in an emergency, free access to the power column at the right side of the instrument must be possible at any time.



Â

Do not block the ventilation slots of the mass spectrometer. Items might fall behind the instrument, inhibit airflow, and cause the system to overheat.

## **Moving the Instrument**

Before you move the instrument from one place to another, all participating personnel must carefully read and follow the instructions given in this manual. For information about moving the forepump, see page 8-11.

The instrument has eight recessed grips at its underside—two at the front side and three at each the left side and the right side. The grips become accessible after the filter brackets are removed. For shipment, the instrument is fixed with two brackets on a pallet. See Figure 5-2.



Figure 5-2. Bracket, fixed on the transport pallet

▲ CAUTION Heavy Load. Because of its weight of about 120 kg, handling the instrument alone might cause muscle strain and back injury. To lift and move the instrument, at least *four persons* are necessary to keep the individual load below acceptable limits (maximum 40 kg for men or 15 kg for women for a duration of 5 seconds). The carriers must be trained in how to carry loads properly (for example, by rising from the knees with a straight back). Thermo Fisher Scientific recommends that you use a pallet jack to lift the mass spectrometer to the height of the workbench.

#### **ACAUTION**

**Heavy Objects.** The mass spectrometer and the forepump might move uncontrollably and cause injuries. Wear steel-reinforced safety shoes and gloves during installation or maintenance.

Considerable space for moving must be available for the four persons that carry the instrument. Therefore, Thermo Fisher Scientific recommends that you use a pallet jack when you move the instrument into another room.

The instructions that follow assume that the instrument has been moved to the installation site with a pallet jack and the top cover of the transport crate has been removed.

#### \* To move the instrument onto the workbench

- 1. Gather four persons and appoint one person that takes command and gives instructions to the remaining people.
- 2. Lift the instrument to the height of the working bench with the pallet jack.
- 3. Remove the two brackets that attach the instrument to the transport pallet. See Figure 5-2.
- 4. Remove the filter brackets on the sides of the instrument. The lifting grips come into view.



Filter bracket



- 5. On command, all four carriers lift off the instrument simultaneously—to prevent them from experiencing an uneven load distribution. Place the instrument onto the bench.
- 6. Only two persons are necessary for moving the instrument into its final position on a bench:
  - a. Rest the rear part of the instrument on the bench and slide it into the correct position. The rear row of the support points below the instrument consists of synthetic material that has a low frictional resistance. It should easily slide above the surface of your workbench.
  - b. When the final position for the instrument is reached, slowly lower the front of the instrument. The front row of the support points below the instrument consists of synthetic material that has a high frictional resistance. It should keep the instrument safely in position.

# **Placing the Forepumps**

The Orbitrap Exploris 480 MS is shipped with a high-throughput source vacuum pump<sup>1</sup> and a low-throughput auxiliary forepump<sup>2</sup>. All other Orbitrap Exploris Series MS use a single-stage rotary vane pump<sup>3</sup> as forepump.

All forepumps come with separate noise reduction covers. Each pump is placed on a drip pan with wheels. Install the pumps on the floor below the workbench. If the workbench has no space below it, place the pumps at the end of the workbench. Before you place the pumps, Thermo Fisher Scientific strongly recommends that you consider the information contained in "Vibration" on page 5-18.

# **CAUTION Heavy Object.** Because of their weight (~80 kg resp. ~60 kg), the large forepumps might move uncontrollably and cause injuries. Wear steel-reinforced safety shoes when you move the pump during the installation.

#### **Connecting the Forepumps**

The vacuum hose of the source vacuum pump has an inner diameter of  $38 \text{ mm} (1\frac{1}{2} \text{ in.})$ . Connect the vacuum hose of the source vacuum pump to the large vacuum port at the left side of the mass spectrometer. See Figure 5-4.

The vacuum hose of the auxiliary forepump of the Orbitrap Exploris 480 MS has an inner diameter of 19 mm (3/4 in.). Connect the vacuum hose of the auxiliary forepump to the small vacuum port at the left side of the MS. Run the auxiliary vacuum hose according to the same instructions as described above for the main vacuum hose. To avoid a vacuum leak, the hose clamp should be positioned only about 2 mm away from the end of the vacuum port, where the metal tube is not curved.

Both vacuum hoses have a length of 2.0 m (79 in.). They are made of reinforced material.

Connect the exhaust hoses of the pumps to the exhaust system of the laboratory. Use the T-piece that is shipped with the Orbitrap Exploris 480 MS to join the exhaust lines of both forepumps.



The maximum length for the exhaust hose of the forepump is 10 m.

<sup>&</sup>lt;sup>1</sup> Leybold SOGEVAC<sup>™</sup> SV 120 BI, or approved equivalent model

<sup>&</sup>lt;sup>2</sup> Pfeiffer DUO 11, or approved equivalent model

<sup>&</sup>lt;sup>3</sup> Leybold SOGEVAC<sup>™</sup> SV 65 BI, or approved equivalent model



Figure 5-4. Vacuum ports of Orbitrap Exploris 480 MS

No.	Description	No.	Description
1	Vacuum port for auxiliary forepump <sup>a</sup>	2	Vacuum port for source vacuum pump

<sup>a</sup> This port is not present in the Orbitrap Exploris 120, Orbitrap Exploris 240, and Orbitrap Exploris MX MSs.

All forepumps are switched on and off by a contact closure signal from the mass spectrometer. Connect the switch cable of the pumps to the D-sub port on the control panel at the right side of the MS. See Figure 3-11 on page 3-21. Connect the power supply cords of the pumps to wall outlets. See page 5-10 for specifications of the power supply.

To prevent an unwanted operation of the forepump, connect the MS and the pump to the power supply in the correct sequence:

- When you install a system, first connect the switch cable between the instrument and the pump, then connect the power supply cords.
- When you deinstall or service a system, first disconnect the power supply cords, then disconnect the switch cable between the instrument and the pump.

The auxiliary forepump of the Orbitrap Exploris 480 MS has a voltage selector switch. Make sure that you have set the correct voltage (115 V or 230 V) before you connect the pump's power supply cord to the wall outlet.



NOTICE

## **Option: Dry Pumps**

Thermo Fisher Scientific offers dry pumps as alternative to the standard forepumps. The dry pumps have these advantages:

- Lower power consumption
- Less air conditioning needed
- Less acoustic noise
- Smaller footprint
- No regular oil exchange (maintenance every four years by the manufacturers)

Table 5-2 shows the correct dry pump for each Orbitrap Exploris Series mass spectrometer. The dry pump for the Orbitrap Exploris 480 MS has two vacuum ports and replaces both forepumps for the MS.

**Table 5-2.**Dry pumps for Orbitrap Exploris Series MS

Instrument	Dry Pumps Model <sup>a</sup>
Orbitrap Exploris 120 MS  Orbitrap Exploris 240 MS, Orbitrap Exploris MX MS	Leybold ECODRY 65 plus
Orbitrap Exploris 480 MS	Edwards nXL110iD

<sup>a</sup> See page 9-3 for part numbers.

Because of the lower noise level, the dry pumps are shipped without noise reduction covers. The tables 5-3 and 5-4 show important properties of the dry pumps.

**Table 5-3.** Space and load requirements of dry pumps

Dry Pump	Noise Level	Hei	ght	Wi	dth	Len	gth	We	ight
	dB(A)	mm	in.	mm	in.	mm	in.	kg	lb
Leybold ECODRY 65 plus	52	287	11 <sup>5</sup> / <sub>16</sub>	320	$12\frac{5}{8}$	600	23 <sup>5</sup> / <sub>8</sub>	43	95
Edwards nXL110iD	57	344	13 <sup>9</sup> / <sub>16</sub>	308	$12\frac{1}{8}$	654	25 <i>3</i> /4	78	172

**ACAUTION** 

**Heavy Object.** Use suitable lifting equipment when you move a pump during the installation. For detailed instructions (maximum tilt angle, for example), refer to the manufacturer's documentation that is shipped with the pumps.

Leybold ECODRY 65 plus					
Nominal voltage	120 V AC	200-240 V AC			
Frequency	60 Hz	50/60 Hz			
Phases	Single				
Rated current	15 A	10 A			
Rated power	1200 VA				
Fuse	15 A (slow blow)	16 A (slow blow)			
Edwards nXL110iD					
Nominal voltage	200–230 V AC, 50/60 Hz, single phase				
Input current	8.5 A				
Fuse	15/16 A (tripping charac	cteristic C)			

Table 5-4.	Electrical	data	of	dry	pump
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# **Laboratory Conditions**

This section gives an overview of important requirements for the laboratory where the Orbitrap Exploris Series mass spectrometer is placed. For details, refer to the *Orbitrap Exploris Series Pre-Installation Requirements Guide*.

#### **Power Supply**

An Orbitrap Exploris Series LC/MS system has the basic power requirements as shown in Table 5-5.

**Table 5-5.**Power Requirements

Mass Spectrometer	
Nominal voltage	208–240 V AC, 50/60 Hz, single phase
Power	apparent power: 800 VA; effective power: 750 W
Fuse <sup>a</sup>	15/16 A (tripping characteristic C)
Source Vacuum Pump	
Nominal voltage	200–240 V AC, 50/60 Hz, single phase
Power	1.5 kW (2.2 kW) <sup>b</sup>
Fuse <sup>a</sup>	15/16 A (tripping characteristic C)
Auxiliary Forepump <sup>b</sup>	
Nominal voltage	115 V or 230 V AC, 50/60 Hz, single phase
Power	0.25 kW (50 Hz) / 0.3 kW (60 Hz)
Fuse <sup>a</sup>	16 A (115 V) / 6 A (230 V), slow
Data System (Computer	; Monitor, and Ethernet Switch) and LC
Nominal voltage	100–240 V AC, 50/60 Hz, single phase
Fuse <sup>a</sup>	15/16 A

Syringe Pump and Switching Valves

The mass spectrometer provides electric power for the syringe pump and the switching valve(s).

<sup>a</sup> dedicated wall outlet

<sup>b</sup> In case of an Orbitrap Exploris 480 MS.

Thermo Fisher Scientific provides country-specific power cords for the mass spectrometer, forepumps, data system, monitor, and Ethernet switch. They are approximately 2.5 m (8 ft) long. One power cord fits into a standard IEC 60320 C19 socket on the source vacuum pump. The other cords fit into standard IEC 60320 C13 sockets on the mass spectrometer and the other system components. Plug the cords into wall outlets.

The power column at the right side of the instrument provides power connections for the mains supply, the syringe pump, and the switching valves. See Figure 5-5.



Figure 5-5. Power column

No.	Description	No.	Decription
1	Holders for power supplies of syringe pump and switching valve	2	Mains supply connector
3	Power supply for syringe pump and switching valves <sup>a</sup>	4	Main Power switch
5	Electronics service switch		

<sup>1</sup> Four outlets for secondary consumers are available on the MS. The total maximum current of the secondary consumers must not exceed 3 A.



Inadequately rated power cords might cause damage to the instrument. If you must replace the cords that are shipped with the instrument, use only original spare parts supplied by Thermo Fisher Scientific.

#### NOTICE

The instrument is tested and certified for a line voltage between 208 V and 240 V. In some areas of the world, voltage sags during high use periods might decrease the working voltage. For nominal voltages below 208 V or for areas with working voltages below 187 V due to voltage sags, you must protect your instrument by using a suitable power conditioner or an uninterruptible power supply (UPS).



**Electric Current.** Electric shock hazard. Incorrect usage of these ports might endanger personnel. Read and understand this manual to prevent harm to the operator and to protect equipment against damage. To make sure that the instrument is free from all electric current, always disconnect the power cords of the *mass spectrometer and the forepumps* before you try any type of maintenance.

#### Voltage Dependency of the Ion Source Heater

The heater of the ion source operates with line voltage. If the main supply voltage drops below its nominal value, the maximum temperature of the heater might not be available anymore. Figure 5-6 shows the derating curve of the maximum vaporizer temperature in dependence of the line voltage and the operating conditions for the HESI source.



Figure 5-6. Maximum vaporizer temperature vs. line voltage

#### **Gas Supply**

The mass spectrometer requires nitrogen gas for the API sheath gas, API auxiliary/sweep gas, reagent carrier gas, C-Trap bath gas, and HCD collision gas. The gas consumption strongly depends on the type of analysis the instrument is used for. It is essential that the gas be delivered with the necessary pressure and purity. See Table 5-6.

Gas type	Pressure	Purity	Tubing OD	Maximum Flow	Consumption
Source gas		99%	6 mm	45 ln/min	65000 ln/day
Reagent carrier gas, C-Trap bath gas, HCD collision gas	0.6 ± 0.05 MPa	99.999% (mandatory)	1/16 in.	0.03 ln/min	40 ln/day

#### **Table 5-6.** Nitrogen supply requirements

#### NOTICE

Your laboratory gas supply may provide nitrogen also for other consumers or peripherals. In this case, make sure that the supply for the MS always meets the requirements for pressure, purity, and stability described in this topic.

The MS can operate reliably only when the pressure of the source gas stays within the required limits. If your laboratory gas supply provides nitrogen also for other consumers, then you must install a pre-regulator in the gas line that leads to the source gas port of the MS.

The gas inlet ports are at the left side of the instrument. See Figure 5-7. The port for source gas & vent gas (top) has a press-in fitting for a 6 mm hose. The port for C-Trap gas & HCD collision gas (bottom) has a Swagelok<sup>™</sup>-type fitting for 1/16 in. tubing.



Figure 5-7. Gas connections at the left instrument side



Do not connect other gases than nitrogen to the mass spectrometer! This might affect instrument performance. The maximum pressure for the gas inlet is 0.65 MPa (6.5 bar, 94 psi).

For the Orbitrap Exploris 120, Orbitrap Exploris 240, and Orbitrap Exploris 480 MSs, the fragment ions that are generated in the ion-routing multipole are generally quite reactive. High purity nitrogen contains notably more water and oxygen than ultra-high purity nitrogen, which gives rise to gas-phase adducts and related products. These species would deteriorate the MS/MS spectral assignments. For the ion-routing multipole, ultra-high purity (UHP, 99.999%) nitrogen

is therefore mandatory.

For the reagent carrier gas, ultra-high purity (UHP, 99.999%) nitrogen is also mandatory.

The gas consumption strongly depends on the type of analysis the instrument is used for. See Table 5-7.

#### Table 5-7. Typical nitrogen consumption of LC/MS applications

Application	LC Flow Rate	Source Settings [arbitrary units]	Consumption [In/min]		
	(approximate)		Source gas <sup>a</sup>	HCD collision gas	
Nano-Spray		sheath gas = 0, aux gas = 0, sweep gas = $0$	0		
Low flow	5 μL/min	sheath gas = 5, aux gas = 0, sweep gas = $0$	7	0.03 <sup>b,c</sup>	
Medium flow	200 µL/min	sheath gas = $35$ , aux gas = $10$ , sweep gas = $0$	15	- 0.05	
High flow	1 mL/min	sheath gas = $60$ , aux gas = $20$ , sweep gas = $5$	28	-	

<sup>a</sup> It is recommended to keep the background gas flow activated (select the check box "Enable Minimum Gas Flow Requirement for Ion Source" in the Instrument Configuration window). See also the Tip concerning the Standby condition.

<sup>b</sup> UHP gas is mandatory.

<sup>c</sup> With the Internal Calibration source in use, the consumption of UHP nitrogen gas increases up to 65 sccm ( $\approx$ 0.07 ln/min). See page 3-19.

Table 5-8 shows the estimated nitrogen consumption for different calibration types at ambient pressure. Low-flow settings are used (source gas consumption:  $7 \ln/\min$ ).

#### **Table 5-8.**Estimated Nitrogen Consumption for a Calibration

Action	Estimated duration	Estimated consumption
Manual spray stability optimization	30 min	195 ln
Mass calibration	1 min	5 ln
Full system calibration <sup>a</sup>	2 hours	800 ln

The values include 30 minutes to ensure a stable spray.

**Tip** When you place the MS in Standby condition, do not switch off the nitrogen supply of the laboratory. An automatic source background flow of nitrogen prevents the backstreaming of contaminants and dust into the instrument:

Instrument	ln/min	ln/day
Orbitrap Exploris 120 MS	2.3	3300
Orbitrap Exploris 240 MS		
Orbitrap Exploris MX MS		
Orbitrap Exploris 480 MS	7	10000

You can supply the nitrogen for your instrument from one source (single supply) or two sources (dual supply). See Table 5-9 for an overview. Figure 5-7 shows an instrument that is completely supplied with

UHP nitrogen (single supply). Make sure that the maximum flow rate of the nitrogen source of your choice matches the requirements of your applications.

Table 5-9.         Gas supply properties for single supply and dual supply	ply
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Supply Type	Nitrogen Pu	rity	Nitrogen Source (Examples)
Single Supply	>99.999%	purity (<0.001% oxygen content)	LN2 evaporator, cylinder bundle, PSA nitrogen generator
Dual Supply	Collision gas:	>99.999% purity (5.0)	LN2 evaporator, cylinder bundle, PSA nitrogen generator
Source		Required: >95% (<5% oxygen content)	Membrane nitrogen generator
	gases:	Recommended: >99% (<0.5% oxygen content)	LN2 evaporator, cylinder bundle, PSA nitrogen generator

#### \* To connect a single nitrogen source to the mass spectrometer

- Connect an appropriate length of Teflon<sup>™</sup> hose to the UHP nitrogen source in the laboratory. The Installation Kit contains 10 m (33 ft) of a suitable hose (OD 6 mm, see Chapter 9, "Replaceable Parts"). The connection for the Teflon hose to the nitrogen gas supply is not provided in the kit. You have to supply this part.
- 2. Insert the opposite end of the Teflon hose into the press-in fitting of the Y-piece that is attached to the gas ports at the left side of the instrument. See Figure 5-7. To connect the hose, align the Teflon hose with the opening in the fitting and firmly push the hose into the fitting until the hose is secure.
- 3. The Y-piece splits the nitrogen flow to source gas and trapping gas. Use a short segment of 6 mm ID hose to connect the Y-piece to the top gas port on the instrument. Use a 6 mm ID to 4 mm union, a 4 mm to 1/16 in. union, a short piece of stainless steel tubing and two sets of fitting and ferrule to connect the Y-piece to the bottom gas port on the instrument.
- \* To connect two nitrogen sources to the mass spectrometer
- 1. Remove the Y-piece with the two short tubing sections from the instrument.
- 2. Connect the 6 mm hose that comes from the *high-purity nitrogen* source to the *top nitrogen inlet* of the instrument.
- 3. Connect the 1/16 in. tubing that comes from the *ultra-high purity nitrogen* source to the *bottom nitrogen inlet* of the instrument.

# Laboratory Temperature

		The mass spectrometer is designed to operate at a laboratory room temperature between 18 and 27 °C (64 and 81 °F).
	NOTICE	Do not put the mass spectrometer below an air duct, near windows, or near heating and cooling sources. Temperature fluctuations of 0.5 °C or more over a period of 10 minutes can affect instrument performance.
		If the temperature in the laboratory has changed for more than 2 °C since the last mass calibration, Thermo Fisher Scientific strongly recommends that you refresh the mass calibration.
		The T1 1 1 water and 1 days at the state of the UUIX
		chamber increases with the temperature in the laboratory. To faster reach the ultimate UHV vacuum, we recommend keeping the laboratory temperature at the lower end of the range.
Humidity		
		The relative humidity of the operating environment must be between 20 and 80%, with no condensation. Thermo Fisher Scientific recommends to install a temperature/humidity monitor in your laboratory. This makes sure that the laboratory is always within the specifications for temperature and humidity.
	NOTICE	Operating the mass spectrometer at very low humidity might cause the accumulation and discharge of static electricity, which can shorten the life of electronic components. Operating the mass spectrometer at high humidity might cause condensation, oxidation, and short circuits, and will also block the filters on the cooling fans.
		A significant change of the humidity in the laboratory can affect the mass accuracy. If the humidity in the laboratory has changed significantly since the last mass calibration, Thermo Fisher Scientific recommends that you refresh the mass calibration.

#### **Ventilation and Fume Exhaust**

The vacuum waste and the solvent waste must be vented separately, and the wastes must be collected and disposed of properly.

Table 5-10.	S١	/stem	waste	and	exhaust	rec	uirements
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Pump exhaust requirements	Inrush flow rate	10 L/min
	Continuous flow rate	7 L/min
Ion source exhaust requirements	Maximum flow rate	45 L/min

Consider the following safety guidelines for ventilation and exhaust. See also "Connecting the Source Housing Drain to the Solvent Waste Container" on page 5-20.

**WARNING** Suffocation Hazard. A significant amount of the nitrogen that is introduced into the API source can potentially escape into the laboratory atmosphere. Accumulation of nitrogen gas could displace sufficient oxygen to suffocate personnel in the laboratory. Make sure that the laboratory is well ventilated. Always operate the instrument with the drain tubing connected to a waste container that is connected to a dedicated fume exhaust system. Local regulations may make a risk assessment for the workplace necessary.

**WARNING** Hazardous Chemicals. The source exhaust might contain noxious material. It will contain traces of the samples and solvents that you are introducing into the source. Potential health hazards of these compounds include chemical toxicity of solvents, samples, and buffers, as well as biohazards of biological samples. To prevent contamination of the laboratory, always operate the instrument with the drain tubing connected to a waste container that is connected to a dedicated fume exhaust system. Do **not** vent the drain tubing (or any vent tubing connected to the waste container) to the same fume exhaust system to which you have connected the forepumps.

#### 

**Hazardous Chemicals.** The forepumps eventually exhausts much of what is introduced into the mass spectrometer, including the small amount of oil vapor that mechanical pumps can emit. The effluent of the forepumps might contain noxious chemicals. Connect the exhaust ports of the forepumps to an exhaust gas line that leads out of the building or to an adequate exhaust system.

**Tip** Organic compounds that are present in laboratory air can contaminate the LC/MS system. They may be the source of background signals in the mass spectrum. Take precautions to keep the laboratory air clean. Prevent airborne contaminants from entering the solvents.

## Vibration

	Floors must be free of vibration caused, for example, by equipment in adjoining locations. Excessive vibration can lead to a reduced lifetime of mechanical components and potentially can have an impact on performance. We recommend to maintain the vibration levels below the levels for office spaces as defined in ISO 9241-6:1999.
NOTICE	Because of the natural vibration of a forepump during operation, it must not have any mechanical contact to the mass spectrometer with the exception of the vacuum hose. Otherwise, the vibration might affect instrument performance. Therefore, install the pump on the floor below the mass spectrometer and not near the system on the workbench.
Altitude	Orbitrap Exploris Series mass spectrometers are designed for indoor use at an altitude of up to 3000 m (10 000 ft) above sea level. To check whether a peripheral (for example, LC or printer) is suitable for the intended altitude, refer to the peripheral's manual or contact Thermo Fisher Scientific.
Airborne Neice Emission	

#### **Airborne Noise Emission**

The A-weighted emission sound pressure level created by the mass spectrometer at work stations does not exceed 70 dB(A).

# Setting Up the Instrument Hardware and Adjusting the System Parameters

Only employees of Thermo Fisher Scientific or personnel who act on behalf of Thermo Fisher Scientific are allowed to install the mass spectrometer.

The mass spectrometer and other devices shipped with it are installed by a Thermo Fisher Scientific field service engineer. During the installation, the service engineer will demonstrate the basics of equipment operation and routine maintenance.

If you wish to connect the mass spectrometer to other LC equipment, see "Connecting Frequently Used Devices" on page 5-23 for advice. Also refer to the manuals that came with the LC equipment.

For detailed information about changing the instrument parameters and developing experiments for the instrument, refer to the Tune Help.

#### **Connecting the Data System and the Mass Spectrometer**

Place the data system workbench and the LC/MS workbench adjacent to each other to prevent strain on the interconnecting Ethernet communications cables. The Ethernet port of the MS is located on the control panel at the right side of the instrument. See Figure 3-11 on page 3-21. Connect the Ethernet cables from the Ethernet switch to the data system computer's LC/MS Ethernet network card and the MS.

# **Configuring the Ion Source**

The API source can be configured to operate in several API modes, which include electrospray ionization (ESI) for calibration only, heated electrospray ionization (HESI), atmospheric pressure chemical ionization (APCI), and atmospheric pressure photoionization (APPI). A separate nanospray ionization (NSI) probe is necessary to operate in NSI mode.

#### **Connecting the Source Housing Drain to the Solvent Waste Container**

The mass spectrometer internally routes the solvent waste from the bottom of the API source to the source drain port. See Figure 3-8 on page 3-17. During the initial installation of the mass spectrometer, a Thermo Fisher Scientific field service engineer installs the solvent waste system. The components of the solvent waste system are contained in the Installation Kit.

Equip your lab with at least two fume exhaust systems:

- The analyzer optics become contaminated if the drain/waste tubing and the exhaust tubing from the forepump connect to the same fume exhaust system. Route the exhaust tubing from the forepump to a dedicated fume exhaust system. See page 5-6.
- Vent the waste container to a dedicated fume exhaust system. The exhaust system for the API source must accommodate a flow rate of up to 45 L/min (95 ft<sup>3</sup>/h).

#### \* To connect the solvent waste container to the MS

1. Connect the venting cap to the solvent waste container, and then connect the waste tubing to the cap openings.



Figure 5-8. Solvent waste connections

- 2. Use the provided Tygon<sup>TM</sup> tubing (1 in. ID,  $1\frac{3}{8}$  in. OD) to connect the solvent waste container to the drain/waste port of the instrument.
- 3. Use the provided black spiral tubing to connect the waste container to the external exhaust system. Make sure that your lab exhaust system can accommodate this tubing (1 in. ID, 1¼ in. OD) without using reducing connectors along the solvent waste path.

To prevent solvent waste from backing up into the instrument, make sure that all tubing is above the level of liquid in the waste container as follows:

- From the MS to the solvent waste container.
- From the waste container to the exhaust system.

**CAUTION** Tripping Hazard. After completing all connections, route the tubing so that they are not a trip hazard.

To prevent the laboratory from being accidentally contaminated by solvent waste, protect the waste container against overturning.

**Tip** The cap adaptor insert of the solvent waste container has a small vent. If the exhaust port of the laboratory is always at negative pressure, Thermo Fisher Scientific recommends that you remove the cap that covers the vent. This makes the atmosphere in the solvent waste container independent of the fume exhaust system.

#### **Changing the Ion Source Housing**

NOTICE

For information about changing the ion source housing, see "Removing and Reinstalling the API Source Housing" on page 8-24. Also refer to the manuals that came with the API source and the API probe. When you change the ion source housing, pay attention to the general safety guidelines that follow.

**WARNING** 

Hazardous Chemicals. The source exhaust might contain noxious material. It will contain traces of the samples and solvents that you are introducing into the source. Potential health hazards of these compounds include chemical toxicity of solvents, samples, and buffers, as well as biohazards of biological samples. To prevent contamination of the laboratory, always operate the instrument with the drain tubing connected to a waste container that is connected to a dedicated fume exhaust system.



**Hot Parts.** During operation of the mass spectrometer, the ion transfer tube and the sweep cone can reach temperatures up to 450 °C. This might cause severe burns upon touching or ignite combustible material. The external surface of the ion source housing can reach temperatures up to 100 °C. This is hot enough to cause skin burns.

Do not touch the ion source housing when the mass spectrometer is in operation. Let the ion source cool down as described in this manual before you remove the ion source housing. Do not touch the ion source mount immediately after you have removed the ion source housing. Keep combustible materials away from the ion source mount. Do not let the instrument stay unattended when the housing is not mounted to the source.

#### **Changing the API Probe**

The mass spectrometer is shipped with the Thermo Scientific OptaMax NG<sup>™</sup> API source housing and a combined HESI/APCI probe. See "API Probe Maintenance" on page 8-34 for instructions about installing and removing this API probe.

For information about changing to other API probes, refer to the manuals that came with the API source and the API probe.



Only qualified laboratory personnel are allowed to change the API probe.

# **Connecting Frequently Used Devices**

This section provides information on how to connect the mass spectrometer to external devices that are frequently used with the instrument. It also describes the specifications for the peripheral control connections. For more detailed information, refer to the manuals that come with the devices.

#### **Connecting the API Probe to the Mass Spectrometer**

All the wiring and gas plumbing for the API source are internal. This means you can install or remove the API source or change the ionization mode (HESI, APCI, or APPI) by changing the spray insert—all without the use of tools.

#### \* To connect the liquid lines to the API probe

- 1. Install the API source housing and the API probe onto the mass spectrometer as described in the manuals that came with the API source and the API probe.
- 2. Install the liquid lines between the switching valve, the LC system, the syringe pump, and the grounding union, as appropriate for your application.

#### Setting Up the Inlet for Direct Infusion

To calibrate the mass spectrometer, use the syringe pump to infuse a calibration solution into the ion source that is equipped with the calibration ESI probe. A suitable syringe pump is shipped with the instrument, see page 9-3. For instructions about establishing power supply and communication between syringe pump and mass spectrometer, see page 5-25.

To introduce sample solution with the syringe pump, connect an infusion line between the syringe pump and the grounding union that is held by the grounding bar of the OptaMax NG<sup>™</sup> API source.

To connect the syringe to the grounding union, follow these procedures:

- 1. Setting Up the Syringe
- 2. Connecting an Infusion Line to the Grounding Union

#### **ACAUTION**

**Hazardous Chemicals.** Samples and solvents might contain toxic, carcinogenic, mutagenic, or corrosive/irritant chemicals. Avoid exposure to potentially harmful materials. Always wear protective clothing, gloves, and safety glasses when you handle solvents or samples. Also contain waste streams and use proper ventilation. Refer to your supplier's Material Safety Data Sheet (MSDS) for proper handling of a particular solvent.

#### Setting Up the Syringe

- To fill the syringe, connect it to the LC union, and insert it into the syringe pump
- 1. Fill a clean, 500-µL syringe with your sample solution.
- Connect a 4 cm (1.5 in.) length of Teflon<sup>™</sup> tubing (0.03 in. ID × 1/16 in. OD) with a fingertight fitting (for a 10-32 receiving port and 1/16 in. OD tubing) and a ferrule to the LC union. See Figure 5-9.
- 3. Insert the needle of the syringe into the segment of Teflon tube. Make sure that the needle tip of the syringe fits readily into the opening in the free end of the Teflon tubing. If necessary, you can make the opening at the end of the tubing larger.



Figure 5-9. Connecting the syringe and the LC union

- 4. Place the syringe into the syringe holder of the syringe pump.
- 5. Squeeze the release button on the syringe pump handle and slowly push the handle forward until it just contacts the syringe plunger.

#### **Connecting an Infusion Line to the Grounding Union**

- To connect an infusion line between the LC union and the grounding union
- Connect a section of red PEEK<sup>™</sup> tubing (infusion line) with a fingertight fitting and ferrule (for a 10-32 conical receiving port and 1/16 in. OD tubing) to the free end of the LC union.
- 2. Connect the other end of the infusion line with a fingertight fitting (for a 10-32 port and 1/16 in. OD tubing) and a ferrule to the grounding union.

Figure 5-10 shows the connection between the grounding union and the LC union made with red PEEK<sup>™</sup> tubing and fingertight fittings.





#### **Establishing Power Supply and Communication for the Syringe Pump**

Before you start connecting the syringe pump, make sure that it is safely placed in the accessories cabinet at the top right side of the mass spectrometer.

- To establish power supply and communication between syringe pump and mass spectrometer
- Use the USB cable of the syringe pump to connect it to a USB port in the accessories cabinet of the mass spectrometer. See Figure 5-11. This allows controlling the syringe pump by the instrument software.



Figure 5-11. USB ports

- 2. Connect the power cord of the syringe pump to a peripheral supply port of the MS in the following order:
  - a. Plug the 24 V power cord of the external power supply into the power port at the rear side of the syringe pump.
  - b. Plug the 230 V power cord of the power supply into a peripheral supply port (labeled Power Out) at the power column of the MS. See Figure 5-12.





- 3. Place the power supply of the syringe pump into one of the holders at the rear side of the MS. See Figure 5-12.
- **Electric Current.** Electric shock hazard. Incorrect usage of switches or contact ports might endanger personnel. Read and understand this manual to prevent harm to the operator and to protect the equipment against damage.

Refer to the Help for details about controlling the syringe pump with the Tune application. Refer also to the manual that came with the syringe pump for further information.

#### Establishing Power Supply and Communication for the Switching Valve(s)

Before you start connecting the switching valve(s), make sure that they are safely placed in the accessories cabinet at the top right side of the mass spectrometer.

**Tip** The IDEX<sup>™</sup> MX Series II<sup>™</sup> switching valves support both, USB and contact closure communication. The valve itself must be properly configured. Use the software tool provided by the IDEX corporation to configure it to USB communication before the first use. If it is not recognized at first use, please fully disconnect and unpower the valve and reconnect it again. To use the USB configured valve for other systems using contact closure operation, the valve must be configured back.

# To establish power supply and communication between switching valve(s) and mass spectrometer

- Connect the USB cable to the mating connector on the back of the switching valve. The USB ports of the mass spectrometer are located in the accessories cabinet of the mass spectrometer. See Figure 5-11 on page 5-25.
- 2. The mass spectrometer provides electric power for the switching valve(s):
  - a. Plug the Universal Power Supply male barrel connector into the female port at the rear side of the switching valve.
  - b. Plug the female connector of the power cord into the Universal Power Supply.
  - c. Connect the power cord of the switching valve to a peripheral supply port (labeled Power Out) at the power column of the MS. See Figure 5-12.
  - d. Place the power supply of the switching valve into one of the holders at the rear side of the MS.

Electric power to the switching valve(s) is controlled by the mass spectrometer.

Refer to the Help for details about controlling a switching valve with the Tune application. Refer also to the manual that came with the switching valve for further information.

# **User I/O Connections**

This section describes the specifications for the identical control connections for two peripherals. Location and function of the peripheral control connections are described in "Control Panel" on page 3-21.



Figure 5-13. Peripheral control connectors

#### **Output Specifications**

The mass spectrometer outputs correspond to the status functions listed below. The outputs are potential-free relay contacts, which are closed when the status indicated by the name is true.

These interchangeable outputs are available:

- Digital Out 1 (Pins 3 and 4)
- Digital Out 2 (Pins 5 and 6)

Figure 5-14 shows the circuit diagram and Table 5-11 lists the specifications of the peripheral control output.





Table 5-11.	Output	circuit	specifications
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Parameter	Value
Contact closed	$R_{on} < 1 \Omega$
Contact open	$R_{off} > 1 \ G\Omega \ (typically)$
Current	$I_{max} = 0.6 A$
Voltage	$V_{max} = 60 V$
Power	$P_{max} = 720 \text{ mW}$

#### **Input Specifications**

The mass spectrometer provides a digital input and an analog input to connect external devices.

The *Digital In* input (Pins 1 and 2) is an input with internal pull-up resistor for connecting external relay contacts or open collector transistors. Start is triggered with the falling edge of input voltage. Figure 5-15 shows the circuit diagram and Table 5-12 lists the specifications of the peripheral control output.





Table 5-12.	Digital In i	nput circuit	specifications
-------------	--------------	--------------	----------------

Parameter	Value
Low level input voltage	$U_{in} < 0.8 V @ 0.75 mA$
High level input voltage	U <sub>in</sub> > 2.0 V

The *Analog In* input (Pins 7 and 8) is a differential input without isolation for connecting external analog voltages. Figure 5-16 shows the circuit diagram and Table 5-13 lists the specifications of the peripheral control output.



Figure 5-16.	Analog	input	equiva	lent	schematic
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Table J-13. Analog input circuit specifications	Fable 5-13.	Analog	input	circuit	specifications
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Parameter	Variable	Value
Input Voltage	$U_{in}$	–10 V +10 V
Input Resistance	R <sub>in</sub>	>200 k $\Omega$ (differential)
Input Resistance	R <sub>in</sub>	>100 k $\Omega$ (ground)

# **Obtaining the Calibration Solution**

The Thermo Scientific<sup>TM</sup> Pierce<sup>TM</sup> FlexMix<sup>TM</sup> Calibration Solution is a mixture of 16 highly pure, ionizable components (mass ranges: 40 to 3000 *m/z*). It is designed for both positive and negative ionization calibration with the Tune application for Orbitrap Exploris Series mass spectrometers and other Thermo Scientific instruments that are powered by Orbitrap<sup>TM</sup> technology.

The Pierce FlexMix Calibration Solution features include:

- Improved mass accuracy—extended mass range improves mass accuracy
- Positive and negative mode calibration—single formulation with extended mass ranges for both ionization calibration modes
- Highly validated—high-quality, rigorously-tested formulation with lot-specific certificates of analysis
- Ready-to-use—reference standard may be directly loaded into a syringe and injected into the instrument
- Stable—store at room temperature for up to 18 months

The Pierce FlexMix Calibration Solution is a ready-to-use formulation that has been optimized for both positive and negative ionization calibration of instruments. The extended range masses (40 to 3000 m/z) improve sensitivity and mass accuracy of Orbitrap mass spectrometers. Additionally, the FlexMix Calibration Solution is manufactured at an ISO 9001 facility and each lot is quality controlled with strict specifications. The stable solution is provided in a leak-proof, high-purity PTFE bottle.

**Table 5-14.** Available calibration solution packages

Product Name	Unit Size	Product Number
Pierce <sup>™</sup> FlexMix <sup>™</sup> Calibration Solution	10 mL	A39239

You can order the calibration solution from www.thermofisher.com or www.fishersci.com. The calibration solution is shipped at ambient temperature. Keep it in a dry, cool and well-ventilated place. Keep it in properly labeled containers. Store it in accordance with local regulations.



**Hazardous Chemicals.** Samples and solvents might contain toxic, carcinogenic, mutagenic, or corrosive/irritant chemicals. Avoid exposure to potentially harmful materials. Always wear protective clothing, gloves, and safety glasses when you handle solvents or samples. Also contain waste streams and use proper ventilation. Refer to your supplier's Material Safety Data Sheet (MSDS) for proper handling of a particular solvent.

#### **Solvents and Modifiers**

For the installation of the instrument, LC/MS grade methanol and water must be available. Solvent modifiers might also be necessary during the installation of some systems. The following solvents are useful in operating and maintaining your instrument:

- Methanol
- Acetonitrile
- Water
- Isopropanol
- Acetic acid (modifier)
- Formic acid (modifier)

Some solvent impurities are transparent to UV/VIS detectors. Therefore, some LC/MS grade solvents might contain contaminants that interfere with the performance of the mass spectrometer. To operate your instrument, choose high purity solvents with minimum contamination.

You can order LC/MS grade consumables from Thermo Fisher Scientific, which are sold under its Fisher Scientific brand. Visit www.fishersci.com. Use only Optima<sup>™</sup> LC/MS grade chemicals for operating your system.

**Tip** Do not filter solvents. Filtering solvents can introduce contamination.

#### **Calibration ESI Probe**

A low-flow ESI probe is shipped with the instrument. Use it exclusively for calibrating the instrument. Do not use it for samples! Keep the calibration probe clean (that is, flush it after use) and store it safely in the sprayer container. **Installation** Obtaining the Calibration Solution
# **Operation**

This chapter describes the checks and cleaning procedures of the Orbitrap Exploris Series system that you should perform every day to ensure the proper operation of your system.

### Contents

- Safety Guidelines for Operation on page 6-2
- Before Operating the System on page 6-3
- Setting the System in Standby Condition on page 6-6
- Shutting Down the System on page 6-7
- Starting Up the System after a Shutdown on page 6-9
- Introducing Sample into the Mass Spectrometer on page 6-11
- Resetting the System on page 6-13
- After Operating the System on page 6-14

# **Safety Guidelines for Operation**

When you operate the Orbitrap Exploris Series system, pay attention to these general safety guidelines.

- **Electromagnetic Radiation.** Parts of the forepump emit electromagnetic radiation. This radiation can interfere with the operation of cardiac pacemakers and implanted heart defibrillators, possibly causing death or serious injury. If you wear these devices, keep at least 30 cm away from the forepump.
- **WARNING Hazardous Chemicals.** The forepump eventually exhausts much of what is introduced into the mass spectrometer, including the small amount of oil vapor that mechanical pumps can emit. The effluent of the forepump might contain noxious chemicals. The connection to an adequate exhaust system is mandatory!
  - **WARNING** Hazardous Chemicals. The source exhaust might contain noxious material. It will contain traces of the samples and solvents that you are introducing into the source. Potential health hazards of these compounds include chemical toxicity of solvents, samples, and buffers, as well as biohazards of biological samples. To prevent contamination of the laboratory, always operate the instrument with the drain tubing connected to a waste container that is connected to a dedicated fume exhaust system.
- **CAUTION** Risk of Eye Injury. The thin, sharp, flexible capillaries are difficult to see against the light. There is a risk of being stabbed or cut when you do work with the capillaries. Wear safety glasses to prevent eye injuries!
- **NOTICE** To ensure safety and proper cooling, always operate the MS with its covers in place. This is also necessary to comply with product safety and electromagnetic interference regulations.

### **Before Operating the System**

Every day before you start analyses, make sure that the instrument is ready for operation with these procedures:

- Checking the Forepumps
- Checking the Nitrogen Supply
- Checking the System Vacuum Levels
- Checking the Disk Space on the Data System
- Checking the Mass Accuracy of the Instrument

**Tip** Accurate results can be obtained only if the system is properly calibrated.

### **Checking the Forepumps**

### \* To check the forepumps before use

Make sure that these conditions are met:

- The forepumps are filled with sufficient oil. Refer to the manual that came with the pump for the location and the usage of the oil fill plug and the oil sight glass.
- The forepumps are connected to the power supply.
- The relay control cable is connected to both the MS and the forepumps.
- The gas ballasts of both forepumps are closed.

### **Checking the Nitrogen Supply**

Check the nitrogen supply on the regulator of the nitrogen gas tank or the liquid nitrogen boil-off tank. Make sure that you have sufficient gas for your analysis. If necessary, replace the tank. Verify that the pressure of nitrogen that reaches the mass spectrometer is at  $0.6 \pm 0.05$  MPa  $(6 \pm 0.5 \text{ bar}, 87 \pm 7 \text{ psi})$ . If necessary, adjust the pressure with the tank pressure regulator.

### 

**Fire Hazard.** Air or oxygen in the ion source could produce a fire when it is combined with volatile solvents and high voltages. Introduce combustible samples and solvents into the instrument only with the nitrogen supply connected to the ion source. Make sure that the nitrogen supply is sufficient for daily operation.

### **Checking the System Vacuum Levels**

For proper performance, the mass spectrometer must operate at acceptable vacuum levels. Operating the system at poor vacuum levels can cause reduced sensitivity and tuning problems. Check your system for air leaks and check the system vacuum levels before you start the first acquisition.

### \* To check the vacuum pressures

Make sure that the Status LED at the front of the mass spectrometer is green, which indicates that the instrument is in operating mode. If the LED is not green, check warnings and messages. See "Vacuum Leak" on page 7-5 for instructions. In the Tune window, a green square () indicates that the readback value is good.

### Checking the Disk Space on the Data System

Periodically 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

- From the Home Page window (which is available by choosing Start > Programs > Thermo Xcalibur > Xcalibur), choose Actions > Check Disk Space to open the Disk Space dialog box. The Disk Space dialog box lists the following:
  - Current drive and directory (for example, C:\Xcalibur\system\programs)
  - Number of MB 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 **Directory**.
- 3. When you have completed this procedure, choose **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.

### **Checking the Mass Accuracy of the Instrument**

Thermo Fisher Scientific recommends that you check the mass accuracy before you start to use the instrument. If the instrument indicates in the Tune window that the calibration parameters are not optimal, Thermo Fisher Scientific recommends that you calibrate the mass spectrometer. Refer to the Help for instructions.

**Tip** *Calibration parameters* are instrument parameters that affect the mass accuracy and resolution. They are independent of the sample.

# Setting the System in Standby Condition

Do not shut down the Orbitrap Exploris Series system completely if you are not going to use it for a short period of time, such as overnight or over the weekend. In that case, you can keep the system in Standby condition.

Thermo Fisher Scientific recommends that you keep the mass spectrometer in Standby condition overnight to provide the best mass accuracy next day.

### \* To place the Orbitrap Exploris Series system in the Standby condition

- 1. Wait until data acquisition, if any, is complete.
- 2. Switch off the flow of sample solution from the LC (or other sample introduction device).

For instructions on how to operate the LC from the front panel, refer to the manual that came with the LC.

- 3. In the Tune window, click the **System Standby** button to put the instrument in Standby condition. The Scanning LED on the front panel of the mass spectrometer changes to yellow when the system is in Standby condition.
- 4. Keep the LC power On.
- 5. Keep the autosampler power On.
- 6. Keep the data system power On.
- 7. Keep the Orbitrap Exploris Series main power circuit breaker switch in the On position.

### NOTICE

Dust can be sucked in through the ion inlet system. To reduce this risk to a minimum, keep an ion source housing installed on the mass spectrometer also during off times and standby times.

**Tip** When you place an Orbitrap Exploris Series MS in Standby condition, do not switch off the nitrogen supply of the laboratory. An automatic source background flow of nitrogen prevents backstreaming of contaminants and dust into the instrument:

Instrument	ln/min	ln/day
Orbitrap Exploris 120 Orbitrap Exploris 240 Orbitrap Exploris MX	2.3	3300
Orbitrap Exploris 480	7	10000

### **Shutting Down the System**

The Orbitrap Exploris Series system must not be shut down completely if you are not going to use it for a short period of time, such as overnight or over a weekend. See "Setting the System in Standby Condition" on page 6-6. This section describes how to shut down the system for a maintenance or service procedure.



Power is removed abruptly when you place the main power circuit breaker switch (see Figure 3-11 on page 3-21) in the Off (O) position. Although no component in the system is harmed, this is not the recommended shutdown procedure to follow.

#### \* To shut down the Orbitrap Exploris Series system

- 1. Wait until data acquisition, if any, is complete.
- 2. Switch off the flow of sample solution from the LC (or other sample introduction device).

For instructions on how to operate the LC from the front panel, refer to the manual that came with the LC.



- 3. In the Tune window, click the **System Off** button to put the instrument in Off condition. All high voltages are shut off, as are the sheath and auxiliary gas.
- 4. Put the main power circuit breaker switch of the mass spectrometer in the Off position.

When the rotational speed of the TMP is reduced sufficiently, power to the vent valve solenoid is shut off. The vent valve opens and the manifold is vented with nitrogen.



**High Voltage.** Hazardous electric voltage that can cause an electric shock is used in the instrument. To make sure that the instrument is free from all electric current, always disconnect the power cords of the *mass spectrometer and the forepump* before you try any type of maintenance.



**Hot Parts.** During operation of the mass spectrometer, the ion transfer tube and the sweep cone can reach temperatures up to 450 °C. This might cause severe burns upon touching or ignite combustible material. The external surface of the ion source housing can reach temperatures up to 100 °C. This is hot enough to cause skin burns.

Do not touch the ion source housing when the mass spectrometer is in operation. Let the ion source cool down as described in this manual before you remove the ion source housing. Do not touch the ion source mount immediately after you have removed the ion source housing. Keep combustible materials away from the ion source mount. Do not let the instrument stay unattended when the housing is not mounted to the source.

If you plan to do routine maintenance or preventive system maintenance on the mass spectrometer only, you do not need to switch off the LC, the autosampler, or the data system. In this case, the shutdown procedure is completed. However, if you do not plan to operate the system for an extended period of time, you might want to switch off the LC, the autosampler, and the data system.



Dust can be sucked in through the ion inlet system. To reduce this risk to a minimum, keep an ion source housing installed on the mass spectrometer also during off times and standby times.

**Tip** An instrument that is shut down still consumes nitrogen because the vent valve is connected to the nitrogen supply of the laboratory. Keeping on the nitrogen flow prevents humidity from contaminating the vacuum system of the mass spectrometer. You may however switch off the nitrogen if your supply is limited.

# Starting Up the System after a Shutdown

To start up the Orbitrap Exploris Series mass spectrometer after it has been shut down (and vented), you must do the following:

- 1. Start up the instrument
- 2. Set up conditions for operation
- \* To start up the Orbitrap Exploris Series system
- 1. Make sure that the main power circuit breaker switch of the MS is in the Off (O) position. The electronics service switch should be in the Operating Mode position.
- 2. Make sure that the power cords of all components of the LC/MS system are plugged into the wall outlets.
- 3. Switch on the data system and the monitor as described in the manuals that came with them. Wait until the operating system of the computer is completely loaded.
- Open the Tune application by choosing Start > All Apps > Thermo Instruments > model x.x > model Tune.

**Tip** The data system must be running before you start up the instrument. The instrument will not operate until software is received from the data system.

- 5. Switch on the nitrogen flow at the tank, if it is off.
- Place the main power circuit breaker switch of the MS in the On (|) position. When you place the main power circuit breaker switch in the On (|) position, the forepumps and the turbomolecular pump are started.

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

a. After the main switch is switched On, the pumps of the mass spectrometer are run up. The Pirani gauge (see "Vacuum System" on page 3-37) monitors the pressure at the forepump.

In a short time, the instrument must indicate a significant pressure decrease. If the threshold pressure is not reached after a preset time, or if the rotation speed of the TMP has not reached at least 80% within 15 minutes, the complete vacuum system is switched off.

b. When the TMP has exceeded 90% of its nominal rotation speed, the instrument will try to start an automatic bake-out for 10 hours heating plus 3 hours cooling.

- c. The Cold Cathode Gauge is switched on at the beginning of the cooling phase. It is then used to monitor the vacuum in the Orbitrap analyzer.
- d. The Status LED on the system panel changes to green when all the following conditions are met:
  - In the Tune application, all LEDs are green.
  - Analyzer temperature is below 45 °C.
  - The TMP frequency has exceeded 90% of its maximum rotation speed.
- e. When the vacuum measured by the Cold Cathode Gauge is better than 1E-8 mbar, the power supplies of the high voltage electronics and the tube heater are switched on.
- 7. If you have an LC or autosampler, start it as is described in the manual that came with the LC or autosampler. If you do not have either, set up your mass spectrometer for operation as described below.

**NOTICE** The instrument will start an automatic bake-out for 10 hours heating plus 3 hours cooling when the turbomolecular pump is at nominal speed. This is typically 10–15 minutes after power up of the instrument. The data acquisition PC needs to be up and running and connected to the instrument.

### To set up your Orbitrap Exploris Series mass spectrometer for operation

- Make sure in the Tune application that the UHV pressure is ≤1E-8 mbar. Also make sure that the FV pressure is in the 2 mbar region (Orbitrap Exploris 120, Orbitrap Exploris 240, or Orbitrap Exploris MX MS) or 3.5 mbar region (Orbitrap Exploris 480 MS). Compare the values of the other parameters in the instrument status window with values that you recorded previously.
- 2. Make sure that the gas pressure is within the operational limits:

Nitrogen:  $0.6 \pm 0.05$  MPa ( $6 \pm 0.5$  bar,  $87 \pm 7$  psi)

3. Continue to set up the instrument for operation. See "Before Operating the System" on page 6-3 for additional information.

# **Introducing Sample into the Mass Spectrometer**

A Thermo Fisher Scientific field service engineer has installed the mass spectrometer and the equipment for introducing sample solution and/or calibration solution (LC or syringe pump) and demonstrated their usage. If you wish to connect the MS to other LC equipment, see "Connecting Frequently Used Devices" on page 5-23 for advice. Also refer to the manuals that came with the LC equipment.

Consider the following safety guidelines when you introduce sample into the mass spectrometer.

- **WARNING** High Voltage. If you touch liquid that leaks from the probe sample inlet while the mass spectrometer is in operation, you might receive an electric shock. Do not tighten the probe sample inlet fitting to eliminate a liquid leak while the mass spectrometer is in operation.
- **WARNING** Hazardous Chemicals. Sample solution that contains noxious compounds might drip out of the ion source housing. Always operate the instrument with the drain tubing connected to a waste container that is connected to a dedicated exhaust system.
- ▲ CAUTION Hazardous Chemicals. Samples and solvents might contain toxic, carcinogenic, mutagenic, or corrosive/irritant chemicals. Avoid exposure to potentially harmful materials. Always wear protective clothing, gloves, and safety glasses when you handle solvents or samples. Also contain waste streams and use proper ventilation. Refer to your supplier's Material Safety Data Sheet (MSDS) for information about the correct handling of a particular compound.

### **Performing Mass Spectrum Measurements**

The mass spectrometer is controlled by a PC running the Xcalibur<sup>™</sup> software suite. The software controls all aspects of the instrument. The main software elements are the control of ion detection and the control of the Orbitrap analyzer. Refer to the Help for information.

Consider the safety guidelines that follow when you perform measurements with the mass spectrometer.

### **WARNING**

**Suffocation Hazard.** A significant amount of the nitrogen that is introduced into the API source can potentially escape into the laboratory atmosphere. Accumulation of nitrogen gas could displace sufficient oxygen to suffocate personnel in the laboratory. Make sure that the laboratory is well ventilated. Always operate the mass spectrometer and the API source with attached drain tubing assembly that connects the source drain to a dedicated exhaust system. Local regulations may make a risk assessment for the workplace necessary.



**Fire Hazard.** Air or oxygen in the ion source could produce a fire when they are combined with volatile solvents and high voltages. Introduce combustible samples and solvents into the instrument only with the nitrogen supply connected to the ion source. Make sure that the nitrogen supply is sufficient for daily operation.

**Tip** Organic compounds that are present in laboratory air can contaminate the LC/MS system. They may be the source of background signals in the mass spectrum. Take precautions to keep the laboratory air clean. Prevent airborne contaminants from entering solvents.

# **Resetting the System**

If communication between the mass spectrometer and data system computer is lost, then it may be necessary to reset the system with the reset button of the mass spectrometer.

### ✤ To reset the system

- 1. Make sure that the mass spectrometer and the data system computer are both powered on and that the mass spectrometer is in Standby condition. See page 6-6 for instructions about placing the instrument to Standby condition.
- 2. To reset the mass spectrometer, press the reset button on the control panel. See Figure 3-11 on page 3-21. When you press the reset button, the following occurs:
  - a. An interruption of the embedded computer causes the CPU to reboot.
  - b. After several seconds, the Status LED changes to yellow to indicate that the data system and the instrument are starting to establish a communication link.
  - c. After several more seconds, the Status LED changes to green to indicate that the data system and the instrument have established a communication link. Software for the operation of the instrument is then transferred from the data system to the instrument.

After three minutes, the software transfer is complete. The System LED is either green to indicate that the instrument is functional and the high voltages are on, or yellow to indicate that the instrument is functional and it is in Standby condition.

**Tip** If resetting the system does not resolve the failure:

- 1. Put the electronics switch into the Service Mode position.
- 2. Wait for about ten seconds.
- 3. Put the electronics service switch back into the Operating Mode position.

# After Operating the System

After operating the mass spectrometer, follow these procedures:

- 1. Flushing the Sample Transfer Line, the Metal Needle, and the API Probe
- 2. Cleaning the Sweep Cone and the Ion Transfer Tube
- 3. Purging the Oil in the Forepumps
- 4. Emptying the Solvent Waste Container

**Tip** Thermo Fisher Scientific recommends that you keep the mass spectrometer in Standby condition overnight to provide the best mass accuracy next day.

### Flushing the Sample Transfer Line, the Metal Needle, and the API Probe

Flush the sample transfer line, the metal needle, and the API probe at the end of a working day or a series of measurements (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.

**Tip** You do not need to flush the inlet components (sample transfer line, sample tube, and spray insert) daily. However, if a mass spectrum shows unwanted contamination peaks, flush the inlet components.

### \* To flush the sample transfer line, the metal needle, and the API probe

- 1. Wait until the data acquisition, if any, is complete.
- Open the Tune application by choosing Start > All Apps > Thermo Instruments > model x.x > model Tune.



- 3. From the Tune application window, click the **System On** button to toggle it from Standby to On. The voltages and gas flows to the API source are switched on.
- 4. Set up the HESI probe as follows:
  - a. In the Tune application window, display the HESI Source window.
  - b. In the HESI Source window, enter **30** in the Sheath Gas Flow Rate text box.
  - c. In the HESI Source window, enter **5** in the Aux Gas Flow Rate text box.
  - d. In the HESI Source window, enter **0** in the Sweep Gas Flow Rate text box.

- e. In the HESI Source window, enter **0** in the Spray Voltage text box.
- f. Click **Apply**.
- 5. Set up and start a flow of 50:50 methanol/water solution from the LC to the API source:
  - Set the Flow Rate to a value that is typical for your experiments.
  - Set the solvent proportions to 50% methanol and water.

# **CAUTION** Hazardous Substance. Methanol is highly flammable and noxious. Keep away from heat, sparks, and flame. Avoid accidental exposure. Use with adequate ventilation. When possible, dilute it with 50% water. Refer to your supplier's Material Safety Data Sheet (MSDS) for information about the correct handling of methanol.

- 6. Let the solution flow through the sample transfer line, the metal needle, and the API probe for 15 minutes. After 15 minutes, switch off the flow of liquid from the LC to the API source. Keep the API source (including the APCI vaporizer, the sheath gas, and the auxiliary gas) on for additional 5 minutes. Stop the LC pump.
- 7. After 5 minutes, place the system in Standby condition as described on page 6-6.

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

Clean the sweep cone (or spray 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 remove and clean the sweep cone and the ion transfer tube at the end of each operating day—after you have flushed the sample transfer line, the metal needle, and the API probe with a 50:50 methanol/water solution from the LC. (See "Flushing the Sample Transfer Line, the Metal Needle, and the API Probe" on page 6-14.) If you are operating the system with nonvolatile buffers in your solvent system or with high concentrations of sample, you might need to clean the sweep cone and the ion transfer tube.

### \* To clean the sweep cone and the ion transfer tube

1. Switch off the flow of liquid from the LC (or other sample introduction device) to the API source.

### **CAUTION**

2. From the Tune application window, click the **System Off** button to switch off the mass spectrometer.

**Hot Parts.** The APCI vaporizer typically operates at 350 to 450 °C and the ion transfer tube typically operates at 250 to 400 °C. This might cause severe burns upon touching. Let the ion source cool down as described in this manual before you touch or remove the vaporizer or the ion transfer tube.

- 3. Remove the API source from the front of the mass spectrometer, as described on page 8-25.
- Use a spray bottle filled with 50:50 methanol/water solution and a lint-free industrial tissue (Kimwipes<sup>™</sup>, for example) to clean contaminants from the accessible surfaces of the ion source chamber.

**Tip** To prevent contamination of the ion optical elements, do not clean the sweep cone or the ion transfer tube with solvent when they are attached to the system.

- 5. Remove the sweep cone (if it is installed):
  - a. Put on a new pair of lint- and powder-free gloves.
  - b. Grasp the outer ridges of the sweep cone and pull the cone straight off the API cone seal. See Figure 6-1.



**Figure 6-1.** Sweep cone removed from the MS mount assembly (illustration similar)

6. Clean the ion transfer tube and the sweep cone (if it is installed). See page 8-28 for instructions.

IOTICE		The sweep cones and the ion transfer tubes of the Orbitrap Exploris 480 MS and the other Orbitrap Exploris Series MSs are different. Do not confuse them when you perform maintenance on several instruments. See page 8-28 for details.
	7.	Reinstall the ion transfer tube.
IOTICE		A protective mechanism prevents the air from entering the vacuum manifold. It requires that you insert the ion transfer tube with a quick and steady motion into the spray cone.
	8.	Reinstall the sweep cone: Carefully align the gas inlet on the sweep cone with the sweep gas supply port (Figure 6-1) in the API cone seal. Firmly press the sweep cone into position.
		Note the location of the sweep gas supply port in the API cone seal. The gas inlet on the sweep cone is placed in this port.
		<b>Tip</b> If the spray cone sits either too tight or too loose, adjust the three ball head spring force screws at the spray cone.

9. Reinstall the API source as described on page 8-25.

### **Purging the Oil in the Forepumps**

Purge (decontaminate) the oil in the forepumps on a regular basis to remove water.

### \* To purge the oil in a forepump

- 1. Switch off the flow of liquid from the LC (or other sample introduction device) to the API source.
- 2. From the Tune application window, click the **System Standby** button to put the mass spectrometer in Standby condition.
- 3. Open the gas ballast valve on the forepump. Refer to the manual that came with the pump for the location and the handling of the gas ballast valve.
- 4. Let the pump run for 30 minutes with the gas ballast valve open.
- 5. After 30 minutes, close the gas ballast valve.

Forgetting to close the gas ballast valve increases the risk of either running dry the oil pump or, when venting, getting oil into the vacuum system!



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

#### \* To empty the solvent waste container

- 1. Check the solvent level in the solvent waste container on a daily basis.
- 2. Empty the solvent waste container if it is necessary. Dispose of the solvent waste in accordance with national and local regulations.

# **Troubleshooting**

This chapter provides information about identifying and solving common problems with Orbitrap Exploris Series mass spectrometers.

### Contents

- Safety Guidelines for Troubleshooting on page 7-2
- Fault Table on page 7-3
- Main Power Failure on page 7-4
- Vacuum Leak on page 7-5
- Failure of UHV Chamber Heating Control on page 7-6
- Turbomolecular Pump is not Running on page 7-7
- Turbomolecular Pump cannot reach full Rate on page 7-7
- Failure of Source Heaters / Tube Heaters on page 7-8

# **Safety Guidelines for Troubleshooting**

When you troubleshoot the Orbitrap Exploris Series system, pay attention to these general safety guidelines.

**WARNING** High Voltage. High voltages that can create an electric shock are used in the instrument. Do not remove protective covers from PCBs. Opening the instrument housing is only allowed for maintenance purposes by Thermo Fisher Scientific personnel. To make sure that the instrument is free from all electric current, always disconnect the power cords of the *mass spectrometer and the forepumps* before you try any type of maintenance.

▲ CAUTION Hot Parts. During operation of the mass spectrometer, the ion transfer tube and the sweep cone can reach temperatures up to 450 °C. This might cause severe burns upon touching or ignite combustible material. The external surface of the ion source housing can reach temperatures up to 100 °C. This is hot enough to cause skin burns.

Do not touch the ion source housing when the mass spectrometer is in operation. Let the ion source cool down as described in this manual before you remove the ion source housing. Do not touch the ion source mount immediately after you have removed the ion source housing. Keep combustible materials away from the ion source mount. Do not let the instrument stay unattended when the housing is not mounted to the source.

▲ **CAUTION** Hot Parts. A forepump in function is hot and some surfaces could reach a temperature higher than 80 °C (176 °F). Touching parts of the forepump might cause burns. Switch off the pump and let it cool down before any intervention. If you must work on a pump that is "still warm from operation," then always wear heat protective gloves.

Service by the customer must be performed only by trained qualified personnel and is restricted to servicing mechanical parts. Service on electronic parts must be performed only by Thermo Fisher Scientific field service engineers.

Do not try to repair or replace any component of the system that is not described in this manual without the assistance of your Thermo Fisher Scientific field service engineer.

# **Fault Table**

If malfunctions on the mass spectrometer occur, you will find possible causes and instructions for repair in Table 7-1.

Problem	Possible Causes	<b>Remedy/Information</b>
Tune application shows bad vacuum	System was vented because of a mains supply failure	page 7-4
	Vacuum leak	page 7-5
Temperature of UHV chamber is higher than expected	UHV chamber heating control has failed	page 7-6
Turbomolecular pump is not running	TMP is switched off because of overheating	page 7-7
Temperature of ion source components is higher than expected	Tube heating control or ion source heater control has failed	page 7-8
Temperature of ion source components is lower than expected	Line voltage has dropped (brownout)	page 7-8
Fore vacuum pressure too low	Ion transfer tube is blocked	page 8-28
Full MS sensitivity is reduced	in tansier tube is blocked	Page 0-20

### **Table 7-1.**Troubleshooting

# **Main Power Failure**

A main power failure has the same consequence as switching off with the main power circuit breaker switch. If the power is available again, the system starts up automatically: the pumps are switched on and the vacuum is created.



The instrument will start an automatic bake-out for 10 hours heating plus 3 hours cooling when the turbomolecular pump is at nominal speed. This is typically 10–15 minutes after power up of the instrument. The data acquisition PC needs to be up and running and connected to the instrument.

If the log file of the data system shows a reboot of the system and the pressure reading in the Tune application shows a bad vacuum, this indicates that the system was vented. In case of frequent but short power failures, Thermo Fisher Scientific recommends that you install an uninterruptible power supply (UPS). If main power failures occur frequently while the system is not attended (for example, in the night), Thermo Fisher Scientific recommends that you install a power fail detector.

# Vacuum Leak

For proper performance, the Orbitrap Exploris Series system must operate at acceptable vacuum levels. You can check the current pressure values in the Tune application window.

#### To check the vacuum levels

- Make sure that the Vacuum LED on the front of the mass spectrometer is green, which indicates that the pressure gauges are within their threshold values. In the Tune window, a green square (
  ) indicates that the readback value is good.
- 2. Compare the current values of the pressures in the vacuum manifold with the values listed in Table 7-2. If the current values are higher than normal, there might be an air leak.

Gauge type	Name in Tune application	Typical values
Pirani	Forevacuum Pressure	about 2 mbar resp. 3.5 mbar, depends on temperature of heated ion transfer tube
Pirani	IRM Pressure	1.1E-2 mbar <sup>a</sup> (on/standby mode), 0E0 (off mode) <sup>b</sup>
Cold cathode	UHV Pressure	< 8E-10 mbar

#### Table 7-2. Typical pressure readings

<sup>a</sup> Value may differ for certain operation modes.

<sup>b</sup> Pressure is below measurable range of gauge.

 If the pressure in the Ultra High Vacuum region is high (above 1E-9 mbar), bake out the instrument for about 10 hours or more. See page 8-12 for instructions on performing a system bake-out.

If the pressure remains high, the system might have an air leak. See below for instructions.

- \* To check the system for major air leaks
- Listen for a rush of air or a hissing sound inside the mass spectrometer.
- Possible causes of a major leak might be a loose or disconnected fitting, an improperly positioned O-ring, a contaminated (by debris) O-ring, or an open valve.
- If you suspect an air leak in the forevacuum region, check the vacuum tube for cracks or slits.
- Also check the clamp that fixes the vacuum tube to the forevacuum port (elbow) of the mass spectrometer. See Figure 3-12 on page 3-23. It might be loose because the forepump was shifted or the vacuum tube is twisted.

- Check that the hose clamps are not placed in a curved region of the vacuum connections.
- Make sure that the top lid of the instrument is properly seated.

If the vacuum tube suddenly falls off, the forevacuum port opens completely. When the TMP is at full rate in that moment, the resulting shock wave from atmospheric pressure to high vacuum might destroy it.

### ✤ To fix an air leak

- 1. Shut down the system. See page 6-7.
- 2. Make a visual inspection of the vacuum system and vacuum lines for leaks.
- 3. Check each fitting and flange on the system for tightness, and tighten the fittings or flanges that are loose.

Do not tighten fittings indiscriminately. Pay particular attention to fittings that have been changed recently or to fittings that have been subjected to heating and cooling.

4. Make sure that the O-rings are clean, and that they and the cover plates of the vacuum manifold are properly positioned.

If you cannot find the location of the leak or tighten the leak yourself, contact your Thermo Fisher Scientific field service engineer.

# Failure of UHV Chamber Heating Control

During general operation of the mass spectrometer, the temperature of the UHV chamber is not regulated. Only during a system bake-out, electric power is supplied to the heating elements of the UHV chamber. If the mass spectrometer does not operate as expected, use the Tune application for error diagnosis. Refer to the Tune Help for details.

If the UHV chamber heating control fails, which protects the system from overheating, shut down the mass spectrometer as described on page 6-7. To prevent permanent damage to components of the mass spectrometer, Thermo Fisher Scientific recommends that you call a Thermo Fisher Scientific field service engineer.



# **Turbomolecular Pump is not Running**

A turbomolecular pump may be switched off because of one of the following reasons:

- Turbomolecular pump is blocked.
- Failure of fans in turbomolecular pump.
- Turbomolecular pump starts up too slow and shuts down after 15 minutes.
- System shuts down 70 seconds after power up.

The turbomolecular pump switches off automatically if it is at risk of getting too hot. This protection prevents the outbreak of a fire and minimizes the risk of destructing the pump.

If the mass spectrometer does not operate as expected, use the Tune application for error diagnosis.

In case of startup issues, check the fore vacuum readbacks. In many cases, a leak causes too high pressure to start up the instrument.

In case of an overheated turbomolecular pump, shut down the mass spectrometer as described on page 6-7. To prevent permanent damage to components of the mass spectrometer, Thermo Fisher Scientific recommends that you call a Thermo Fisher Scientific field service engineer.

### **Turbomolecular Pump cannot reach full Rate**

After the mass spectrometer was started, the TMP might not reach the full rate of 1000 Hz. The TMP then stops in about 20 minutes after start.

A possible reason might be that the internal time limit (currently 15 minutes) for the TMP startup is reached. In many cases, a leak causes too high pressure to start up the instrument:

- Double check if the lid of the vacuum chamber is properly seated.
- Check if the inner cage is fully inserted.
- Check if the vacuum hoses are properly connected.
- Check the oil level of the fore vacuum pumps.

Try to start the mass spectrometer again. If the failure of the TMP startup occurs a second time, first check for a vacuum leak and then refer to the other troubleshooting section.

# Failure of Source Heaters / Tube Heaters

A failure of the source heater control or ion transfer tube heater control might lead to an overheating of ion source parts. Non-metallic parts of the ion source (gaskets, for example) are made of non-flammable materials, thus preventing any ignition.

If the mass spectrometer does not operate as expected, use the Tune application for error diagnosis. Refer to the Tune Help for details.

A lasting contrast between the target temperatures set in the Tune application and the observed temperature of hardware components indicates a failure of the heater control. But see also Figure 5-6 on page 5-12 and the accompanying text about the dependency of the transfer tube temperature on the mains supply voltage.

In case of a failure of the source heater control or the tube heater control, shut down the mass spectrometer as described on page 6-7. To prevent permanent damage to components of the mass spectrometer, Thermo Fisher Scientific recommends that you call a Thermo Fisher Scientific field service engineer.

# Maintenance

This chapter describes routine maintenance procedures that must be performed to ensure optimum performance of the Orbitrap Exploris Series mass spectrometer.

### Contents

- Safety Guidelines for Maintenance on page 8-2
- Guidelines for Maintenance on page 8-3
- Inspection- and Servicing Plan on page 8-4
- Tools and Supplies on page 8-8
- Maintaining the Vacuum System on page 8-10
- Maintenance of the Fan Filters on page 8-14
- Maintenance of the Internal Calibrant Discharge Source on page 8-16
- Maintenance of the API Source on page 8-23
- Maintaining LCs or Autosamplers on page 8-43
- Consumables on page 8-43
- Thermo Fisher Scientific Service on page 8-44

# **Safety Guidelines for Maintenance**

When you do maintenance on the Orbitrap Exploris Series system, pay attention to these general safety guidelines:

**WARNING** High Voltage. High voltages that can cause an electric shock are used in the instrument. Do not remove protective covers from PCBs. Opening the instrument housing is only allowed for maintenance purposes by Thermo Fisher Scientific personnel. To make sure that the instrument is free from all electric current, always disconnect the power cords of the *mass spectrometer and the forepumps* before you try any type of maintenance.

▲ CAUTION Hazardous Chemicals. Samples, solvents, and detergents might contain toxic, carcinogenic, mutagenic, or corrosive/irritant chemicals. Avoid exposure to potentially harmful materials. Always wear protective clothing, gloves, and safety glasses when you handle solvents or samples. Also contain waste streams and use proper ventilation. Refer to your supplier's Material Safety Data Sheet (MSDS) for information about the correct handling of a particular compound.

**CAUTION Risk of Eye Injury.** The thin, sharp, flexible capillaries are difficult to see against the light. There is a risk of being stabbed or cut when you do work with the capillaries. Wear safety glasses to prevent eye injuries!

It is the customer's responsibility to maintain the system properly by performing the system maintenance procedures on a regular basis.

Service by the customer must be performed only by trained qualified personnel and is restricted to servicing mechanical parts. Service on electronic parts must be performed only by Thermo Fisher Scientific field service engineers.

Do not try to repair or replace any component of the system that is not described in this manual without the assistance of your Thermo Fisher Scientific field service engineer. Thermo Fisher Scientific assumes no responsibility and will not be liable for instrument damage and/or operator injury that might result from any servicing other than that contained in this manual or related manuals.

## **Guidelines for Maintenance**

Preventive maintenance must start with installation, and it must continue during the warranty period to maintain the warranty. Thermo Fisher Scientific offers maintenance and service contracts. Contact your local Thermo Fisher Scientific representative for more information. Routine and infrequent maintenance procedures are listed in Table 8-1.

Accurate results can be obtained only if the system is in good condition and properly calibrated.

### ✤ To prepare the work area

Do the following:

- Make sure that the surrounding area is neat and clean.
- Prepare a clean work surface by covering the area with lint-free paper or a large sheet of clean aluminum foil.
- Have nearby the necessary tools, supplies, and replacement parts (when applicable).

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

- Always wear a new pair of lint- and powder-free gloves when handling internal components. Do not reuse gloves after you remove them because the surface contaminants on them recontaminate clean parts. See "Personal Protective Equipment" on page 4-14 for a specification for the gloves.
- Always place the components on a clean, lint-free work surface.
- Dirty tools can contaminate your system. Keep the tools clean and use them exclusively for maintenance and service work at the mass spectrometer.
- Do not insert a test probe (for example, an oscilloscope probe) into the sockets of female cable connectors on PCBs.
- Do not overtighten a screw or use excessive force.



Make sure that you do not introduce any scratches or surface abrasions while you handle the internal components. Even small scratches can affect performance if they are close to the ion transmission path. Do not use tools, such as metal pliers, that might scratch these components.

# **Inspection- and Servicing Plan**

Routine and infrequent maintenance procedures to be performed by the user are listed in Table 8-1. For a list of maintenance procedures that must be performed by Thermo Fisher Scientific personnel, see page 8-44.

 Table 8-1.
 User maintenance procedures

MS Component	Procedure	Frequency	Procedure Location	
Instrument	System bake-out	After the system was vented (even partially by a short power outage).	page 8-12	
	Check warning labels on instrument	Annually	page 8-6	
	Leak check gas lines	Annually	page 8-6	
	Check condition of tubings and hoses	Annually	page 8-7	
Cooling fans	Check fan filters	Every four weeks.	page 8-14	
	Clean fan filters	If necessary.	-	
Ion optics	Clean flatapole focus lens	If necessary.	page 8-39	
	Clean injection filter	If necessary.	page 8-37	
	<b>Tip</b> For instructions about performing maintenance on the quadrupole and the bent flatapole, refer to the <i>Orbitrap Exploris Performance Maintenance Manual</i> .			
IC source	Replace	If necessary.	page 8-16	
API source	Flush (clean) sample transfer line, metal needle, and API probe	Daily	page 6-14	
	Clean the sweep cone and the spray cone	Daily	page 6-15	
	Remove and clean ion transfer tube	Daily, or if ion transfer tube bore is contaminated (chemical noise) or obstructed (pressure decrease).	page 8-28	
	Replace ion transfer tube	If ion transfer tube bore is corroded.	page 8-28	
	Clean ion funnel/S-lens	Check bi-weekly. Clean as needed. <sup>a</sup>	page 8-40	
HESI probe	Replace needle insert	If metal needle is blocked.		
APCI, ESI, or HESI probe	Replace metal needle	If metal needle is broken or obstructed.	See manufacturer's documentation.	
Calibration ESI probe	Replace low-flow needle assembly	If metal needle is blocked.		

MS Component	Procedure	Frequency	Procedure Location	
Forepump	Purge (decontaminate) oil	Daily <sup>b</sup>	page 6-17, see also manufacturer's documentation	
	Check oil level	Daily	page 8-10, see also	
	Check oil condition	Depends on process.	manufacturer's	
	Add oil (requires venting)	If oil level is close to minimum.		
	Check filter insert of external oil mist filter	Daily	-	
	Check gas ballast valve	Monthly	-	
	Change oil	Every 8000 h (~one year) of operation.	-	
	Replace exhaust filter	If oil mist appears at exhaust or annually.	_	
	Check anti-suckback valve	Annually	-	
	Clean fan cover	Annually	-	

**Table 8-1.**User maintenance procedures, continued

<sup>a</sup> 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.

<sup>b</sup> Depends on the types and amounts of samples and solvents that are introduced into the instrument. For low flow applications, purging the forepump is rarely necessary.

### **Cleaning the Surface of the Instrument**

Clean the outside of the instrument with a dry cloth. To remove stains or fingerprints on the surface of the instrument (panels, for example), slightly dampen the cloth (preferably made of microfiber) with distilled water.



Prevent any liquids from entering the inside of the instrument. Leaking liquids might get into contact with electronic components and cause a short circuit.

### **Checking the Warning Labels**

Safety warnings on the mass spectrometer and other devices of the LC/MS system must always be complete, clearly visible and legible.

In addition to the safety instructions that can be found throughout this manual, warning labels on the instrument inform the user about possible hazards (for example, caused by hot surfaces or high voltage). See "Safety Symbols on the Instrument" on page 4-3 for an overview. To protect all personnel coming near the instrument, annually make sure that all warning labels on the instrument are still present. If warning labels are missing or unreadable, contact a Thermo Fisher Scientific field service engineer for replacements. Also check the warning labels on the forepumps and other devices of the LC/MS system.

### Leak-Checking the Gas Lines

Regularly leak check each gas line from the gas supply in the laboratory to the instrument. The instrument must be powered for the test.

### $\star$ To perform a leak check for a gas line

- 1. After you have closed all valves in the instrument, monitor the manometer of the gas regulator for some minutes.
- 2. If the pressure falls significantly (for example, the nitrogen pressure falls by more than 690 mbar [10 psi] in two minutes), then you should search for leaks in the gas line.
- 3. Search for leaks in the gas line (for example, with a conventional thermal conductivity-based leak detector, such as is widely used to check leaks in gas chromatography equipment).
- 4. If you detect a leak (which is usually at a connection), then verify the tightness of the connection. In case of doubt, replace it. Note that over-tightening a connection might also cause a leak or worsen it.

5. When you cannot find a leak in the gas line, Thermo Fisher Scientific recommends that you call a Thermo Fisher Scientific field service engineer to check for gas leaks in the instrument.

### **Checking the Condition of Tubings and Hoses**

Regularly inspect all tubings and hoses that are connected to the mass spectrometer for damage.

### \* To check the condition of tubings and hoses

- 1. Make sure that the gas lines are securely connected, free from kinks, and not trapped.
- 2. Make sure that the liquid can run freely down the drain tube, which must not contain kinks or liquid traps.
- 3. Visually inspect all tubing for leaks or signs of deterioration.
- 4. Visually inspect the surfaces below all liquid lines for signs of liquid.

If you detect a leak or other damage to any tubing or hose, then you must replace it.

# **Tools and Supplies**

Very few tools are necessary to perform routine maintenance for the Orbitrap Exploris Series MS. You can remove and disassemble many of the components by hand. Table 8-2 lists the necessary chemicals, tools, and equipment for maintaining the instrument.

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

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

Description	Comments
Chemicals	
Isopropanol, methanol, or ethanol	LCMS grade
Water	LCMS grade or ultrapure deionized water, for example Milli-Q $^{\mbox{\tiny TM}}$
Alkaline detergent	For example, Mucasol <sup>™</sup> or Decon 90 <sup>™</sup>
Neutral detergent	For example, Liquinox <sup>™</sup>
Nitrogen gas or compressed air	Clean and oil-free
Tools	
Ion transfer tube removal tool	Provided in the Source Installation Kit
Screwdriver, slot head	
Screwdriver, Phillips #2 (M3)	
Equipment	
Forceps or tweezers	
Magnifying device	
Ultrasonic bath	Ideally heatable
Gloves	Lint-free and powder-free

### Table 8-2. Chemicals, tools, and equipment, continued

Description	Comments
Chamois-tipped swabs	
Lint-free foam tip swabs	
Lint-free wipes	Cleanroom wipes
Polishing paste	For example, 1 µm grain size diamond paste
Polishing linen	For example, MICRO-MESH <sup>™</sup> 6000 and 12000 universal mesh
Blow gun	Supplied with the Cleaning Kit

# **Maintaining the Vacuum System**

This section describes user maintenance procedures for the vacuum pumps and the vacuum manifold of the Orbitrap Exploris Series mass spectrometer.

This section only outlines the maintenance procedures for the forepump and the turbomolecular pump (TMP) of the mass spectrometer. The manuals of the pump manufacturers give detailed advice regarding safety, operation, maintenance, and installation. Note the warnings and precautions contained in these manuals!

### **Maintenance of the Forepumps**

For the forepumps, several maintenance procedures must be performed by the user. See Table 8-1 on page 8-4. To simplify the maintenance work, the pump manufacturer recommends that you combine several jobs. For maintenance instructions, refer to the manual that came with the forepump.

WARNING
 Electromagnetic Radiation. Parts of the forepump emit electromagnetic radiation. This radiation can interfere with the operation of cardiac pacemakers and implanted heart defibrillators, possibly causing death or serious injury. If you wear these devices, keep at least 30 cm away from the forepump.
 Hot Parts. The forepump in function is hot and some surfaces could

**AUTION** Hot Parts. The forepump in function is hot and some surfaces could reach a temperature higher than 80 °C (176 °F). Touching parts of the forepump might cause burns. Switch off the pump and let it cool down before any intervention. If you must work on a pump that is "still warm from operation," then always wear heat protective gloves. Take note of the warning labels on the pump.

# **CAUTION** Hot Liquid. Touching hot forepump oil might cause burns. Always wear protective gloves and protective goggles when you handle the forepump oil.

▲ **CAUTION** Hazardous Chemicals. The forepump oil might cause skin or eye irritation and it might contain toxic, carcinogenic, mutagenic, or corrosive/irritant chemicals. Avoid exposure to potentially harmful materials. Always wear protective clothing, gloves, and safety glasses when you handle the forepump oil.

When you dispose used oil, observe the relevant environmental regulations! For instructions about proper handling, refer to the Material Safety Data Sheet (MSDS) for the forepump oil.
Forepump oil and exhaust filters are available from Thermo Fisher Scientific, see Chapter 9, "Replaceable Parts." If you wish to order other spare parts, contact the pump manufacturer.



To prevent an unwanted operation of the forepumps, connect the MS and the forepumps to the power supply in the correct sequence:

- When you install a system, first connect the switch cable between the instrument and the forepumps, then connect the power supply cords.
- When you deinstall or service a system, first disconnect the power supply cords, then disconnect the switch cable between the instrument and the forepumps.

#### **Moving the Source Vacuum Pump**

For easy and effortless transportation of the source vacuum pump, Thermo Fisher Scientific provides a mobile base (drip pan with casters) with the Orbitrap Exploris Series mass spectrometer.

# **CAUTION Heavy Objects.** The mass spectrometer and the forepump might move uncontrollably and cause injuries. Wear steel-reinforced safety shoes and gloves during installation or maintenance.

The source vacuum pump is heavy (~80 kg resp. ~60 kg). If lifting of the pump becomes necessary, only a suitable lifting device shall be used to lift the pump at the lifting lug.

A lifting device is the only officially recommended way of handling the pump!

Should people lift the pump, at least two persons should lift it. Pay attention to the persons' positions when lifting! Straight back, flexed knees, and adapted large back belts, etc. are recommended.

When you move the pump, obey these guidelines:

- 1 person stands on the left side, one hand below the oil casing and one hand below the pump stator.
- 1 person stands on the right side, one hand below the oil casing and one hand below the motor fan cover.
- Be careful with your hands when you set down the pump into the drip pan to avoid squashing them!

#### NOTICE

Do not lift or pull the pump at the frequency converter or the cables!

### Maintenance of the Turbomolecular Pump

The pump manufacturer recommends that you change the operating fluid reservoir every four years at the latest. Depending on the operating conditions, changing in two-year intervals might be necessary. Changing of the TMP bearing is recommended every four years, at least.

To do maintenance for the TMP, it is necessary to remove the instrument housing and to partially disassemble the instrument. Therefore, a Thermo Fisher Scientific field service engineer must be called if TMP maintenance is necessary. See also page 8-44.

### **Baking Out the System**

The system bake-out of the mass spectrometer removes unwanted gases or molecules (collected or remaining) from the high-vacuum region of the instrument. A bake-out is mandatory after the system has been vented for maintenance or service work in the analyzer region. You should bake out an instrument that has been vented for at least ten hours before you can start using it again.

If the system has been vented during a power failure, then it is necessary to bake out the system to attain the operating vacuum. See "Starting Up the System after a Shutdown" on page 6-9. Before you start the bake-out, make sure that the pumps are up and running at their operating speed. If you have just switched on the mass spectrometer, this will take about ten minutes.

Always check the fore vacuum pressure after switching on the instrument. It should be close to the value shown in Table 8-3 on page 8-13. If the vacuum requirements are not met, the system might self-shutdown again or not start the bakeout procedure to protect itself from damage.

### NOTICE

The instrument will start an automatic bake-out for 10 hours heating plus 3 hours cooling when the turbomolecular pump is at nominal speed. This is typically 10–15 minutes after power up of the instrument. The data acquisition PC needs to be up and running and connected to the instrument.

#### To perform a manual system bake-out

- 1. When the vacuum pressures become normal, place the MS in Off mode in the Tune application window.
- Click the Diagnostics icon ( ), and then choose System > Vacuum > Bake Vacuum Chamber.

- 3. Click **Start**. The MS indicates an active bake-out procedure by a white flashing Status LED and a white progress bar of the Scan LED.
- 4. In the Tune window, do the following:
  - a. Place the MS in **Standby** condition.
  - b. Open the Status pane, click the downward arrow, and then choose **By Board**.
  - c. Check the readback values for the source and Orbitrap (UHV) pressure gauges as follows:
    - Click **Source**, and then verify that the Forevacuum Pressure readback value is below the operating threshold limit (see Table 8-3).
    - Click **FT Vacuum**, and then verify that the UHV Pressure readback value is below the operating threshold limit.

<b>Table 8-3.</b> Typical pressure readings after bake-
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Name in Tune application	Typical values
Forevacuum Pressure	2 mbar resp. 3.5 mbar
IRM Pressure	1.1E-2 mbar
UHV Pressure	<e-10 mbar<="" td=""></e-10>

In the Tune window, normal readback measurements show a green square (
).

### **CAUTION**

**Hot Parts.** If you abort a system bake-out, parts of the instrument can be hot. Touching hot parts of the instrument immediately after a bake-out might cause burns. Let the instrument cool for at least three hours before you start to operate it again.

### **Maintenance of the Fan Filters**

Each of the ventilation slots at the front side, the left side, and the right side of the mass spectrometer is equipped with a fan filter. See Figure 8-1.



Figure 8-1. Fan filter (example)



Do not block the ventilation slots of the mass spectrometer. Items might fall behind the instrument, inhibit airflow, and cause the system to overheat.

**Checking the Fan Filters** 

Check the fan filters every four weeks and clean them if they are dirty. Replacements for the fan filters are available from Thermo Fisher Scientific.

#### \* To check the fan filters

 Each fan filter bracket is plugged into the instrument frame. Beginning at the front side of the instrument, insert a finger into the recess in the bracket and pull at the fan filter bracket to open it. See Figure 8-1 and Figure 8-2.



Figure 8-2. Removing a fan filter bracket

- 2. Pull each fan filter out of the filter bracket and check it for dust. If the fan filters are covered with dust, continue with step 3. If the fan filters are clean, proceed to step 6.
- 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 let them air dry.
- 6. Reinstall the fan filters in the fan filter brackets.
- 7. Reinstall the filter brackets, finishing with the filter bracket at the instrument's front side.

### **Maintenance of the Internal Calibrant Discharge Source**

Over time, the ion signal from the Internal Calibrant discharge source decreases as the internal components become dirty, need to be recalibrated, or both. The expected lifetime of the Internal Calibrant discharge source is six months to one year.

NOTICE

You can service (replace) the Internal Calibrant discharge source, but you cannot service the calibrant vial.

Replace the Internal Calibrant discharge source when the Orbitrap<sup>™</sup> mass analyzer cannot lock to the internal calibrant mass and the S/N of the calibrant peak is less than 33 at a resolution setting of 240000. (Assumes that the instrument has had a full calibration in positive mode, negative mode, and IC modes, and that the mass accuracy of the Orbitrap analyzer is within specification.)

### **Replacing the Internal Calibrant Discharge Source**

The Internal Calibrant discharge source is a consumable part. You may, however, clean the parts that are described in "Cleaning the Calibrant Ion Source" on page 8-20. To replace the Internal Calibrant discharge source, follow these procedures:

- 1. Shut down the mass spectrometer completely, see page 6-7.
- 2. Remove the ion source interface, see page 8-36.
- 3. Remove the Internal Calibrant discharge source, see below.
- 4. Install the new Internal Calibrant discharge source, see page 8-18.
- 5. Reinstall the ion source interface, see page 8-42.
- Before you continue, read the "Safety Guidelines for Maintenance" on page 8-2 and the "Guidelines for Maintenance" on page 8-3. Also take the instructions in "Ion Source Interface Maintenance" on page 8-35 as guidelines.

**Tip** Wear a new pair of lint- and powder-free gloves when you handle API source components. See "Personal Protective Equipment" on page 4-14 for a specification for the gloves.

#### **Removing the Internal Calibrant Discharge Source**

To remove the Internal Calibrant discharge source, follow these procedures:

1. Remove the IC source heater interface.

2. Remove the Internal Calibrant discharge source.

#### \* To remove the IC source heater interface

- 1. Remove the ion source interface (see page 8-36).
- 2. Insert a flat head screwdriver through the holes in the PEEK holder of the injection filter and loosen the screws that attach the injection filter to the ion source interface cage. See Figure 8-18 on page 8-38. Remove the injection filter.
- 3. Continue to loosen the two thumbscrews and use them to carefully pull out the ion funnel/S-lens assembly from the ion source interface cage.
- 4. Loosen the two thumbscrews even further and use them to pull out the IC source heater interface (Figure 8-3).

Hold the heater interface with the thumbscrews facing upward to prevent the calibrant ion source from falling out of the IC source heater interface.



Figure 8-3. Front of the IC source heater interface

#### \* To remove the Internal Calibrant discharge source

1. Hold the IC source heater interface with the thumbscrews facing up.

2. From the bottom, press upward with your fingers to remove the Internal Calibrant discharge source retainer and the Internal Calibrant discharge source (Figure 8-4).



**Figure 8-4.** Calibrant ion source removed from the IC source heater interface

No.	Description	No.	Description
1	Internal Calibrant discharge source retainer	2	Internal Calibrant discharge source
3	Guide pin	4	Orientation notch
5	Orientation tab		

To dispose of the old Internal Calibrant discharge source, see "WEEE Compliance" on page A-3.

#### Installing the New Internal Calibrant Discharge Source

To install the Internal Calibrant discharge source, follow these procedures:

- 1. Install the new Internal Calibrant discharge source.
- 2. Reinstall the S-lens or ion funnel and the IC source heater interface.
- 3. Reinstall the S-lens assembly or ion funnel assembly.

#### \* To install the new Internal Calibrant discharge source

1. Make sure that the discharge cathode is fully inserted into the ceramic insulator (Figure 8-5).

2. Align the Internal Calibrant discharge source and the Internal Calibrant discharge source retainer as shown in Figure 8-4 on page 8-18. Then reinstall them into the IC source heater interface.



Figure 8-5. Calibrant ion source (front view)

- 3. Make sure that the orientation tab of the Internal Calibrant discharge source retainer fits into the corresponding notch in the Internal Calibrant source heater interface.
- \* To reinstall the ion funnel/S-lens and the IC source heater interface
- 1. Align the guide pin on the IC source heater interface (Figure 8-4 on page 8-18) with the guide pin socket on the S-lens or ion funnel, and then firmly press the heater interface until it snaps into place.
- 2. Tighten the two thumbscrews a few turns into the S-lens or ion funnel.
- 3. Carefully slide the S-lens or ion funnel into the ion source interface cage. Compare to Figure 8-20 on page 8-40.
- 4. Tighten the two thumbscrews a few turns into the ion source interface cage.
- \* To reinstall the injection filter

With a slotted screwdriver, attach the injection filter back to the ion source interface cage with the screws.

### **Reinstalling the Ion Source Interface**

- \* To reinstall the ion source interface
- 1. Orient the ion source interface with the release latch at the top. See Figure 8-16 on page 8-36.
- 2. Carefully insert the ion source interface into the vacuum manifold.
- 3. Reinstall the ion source interface housing as described on page 8-25.

4. Start up the system as described in "Starting Up the System after a Shutdown" on page 6-9.

### **Cleaning the Calibrant Ion Source**

When you remove the API source interface from the instrument to clean the internal components, Thermo Fisher Scientific recommends that you also clean the areas of the calibrant ion source as noted in this section.

**Tip** You do not need to remove the calibrant ion source retainer or the calibrant ion source from the IC source heater interface to clean the designated areas.

#### \* To clean the calibrant ion source

- 1. Follow the procedure "To remove the IC source heater interface" on page 8-17.
- 2. Soak foam-tipped swabs in a 50:50 solution of methanol/water.
- 3. Clean the front of the IC Source heater interface with the swabs, as shown in Figure 8-6.



Figure 8-6. Front of the IC Source heater interface

4. On the back of the IC Source heater interface, insert a swab through the calibrant ion source retainer into the opening of the anode ion volume (Figure 8-7), and then clean inside the opening.





- 5. Dry the component with nitrogen gas to make sure that all the solvent evaporates. Also purge through the gas connection at the top (facing front in Figure 8-7).
- 6. Using a magnification device, inspect the opening for any residual lint or particulates.

**Tip** Inspect the inside surface and edges to confirm that no lint or particulates are present. Use plastic tweezers or a similar tool to remove the lint or particulate.

- 7. Follow these procedures:
  - a. "To reinstall the ion funnel/S-lens and the IC source heater interface" on page 8-19.
  - b. "To reinstall the injection filter" on page 8-19.
  - c. "To reinstall the ion source interface" on page 8-19.

### Fluoranthene

The Orbitrap Exploris Series/IC system uses fluoranthene as the calibrant species.





The factory installs 0.15 g of fluoranthene, which is contained in a stainless steel vial, in the calibrant oven assembly. With continuous operation of the mass spectrometer, the calibrant is estimated to last for at least one year. Contact your local Thermo Fisher Scientific field service engineer when it is time to replace the calibrant vial. Only a Thermo Fisher Scientific field service engineer can order and replace the calibrant vial.

Fluoranthene is potentially hazardous. Use it in accordance with its Material Safety Data Sheet (MSDS).

Store and handle all chemicals in accordance with standard safety procedures. The Material Safety Data Sheet (MSDS) describing the chemicals being used should be freely available to lab personnel for them to examine at any time. Material Safety Data Sheets (MSDSs) provide summarized information on the hazard and toxicity of specific chemical compounds.

MSDSs also provide information on the proper handling of compounds, first aid for accidental exposure, and procedures for cleaning spills or dealing with leaks. Producers and suppliers of chemical compounds are required by law to provide their customers with the most current health and safety information in the form of an MSDS. Read the MSDS for each chemical you use. Dispose of all laboratory reagents in the appropriate manner (see the MSDS).

### **Maintenance of the API Source**

Various routine maintenance procedures must be performed to ensure the optimum performance of the Atmospheric Pressure Ionization (API) source. Most of the procedures involve cleaning. This section also describes procedures for replacing the ion transfer tube. Refer also to the *OptaMax NG Ion Source User Guide* for additional information.

#### **Cleaning Environment**

Before you open the system to perform cleaning, prepare a clean, sufficiently large surface that is covered by a clean metal tablet or a sheet of sturdy aluminum foil, free of dust and particles. Always wear clean gloves when you handle parts that are removed from the vacuum manifold. All tools that are used in the vacuum manifold should be clean, and free from oil, particles, and dust. All devices, holders, lenses, etc. that are removed from the vacuum manifold should be placed on the clean surface. Keep the vacuum manifold closed when it is not actively being accessed. Likewise, cover removed parts to prevent dust accumulation when they are not actively being accessed.

#### **Using Abrasives**

### NOTICE

Use abrasives only when it is absolutely necessary or as a last resort to remove problematic stains. When you use abrasives (polishing paste or MICRO-MESH<sup>™</sup>), either thoroughly wipe off the generated particles with lint-free wipes (first wet, then dry) or rinse them off with water. Most lenses are easy to wipe, while other ion optics parts should be rinsed. Always add some solvent to prevent dry particles from spreading on the cleaned surface.

#### **Cleaning Solutions**

Prepare these cleaning solutions:

- 2% alkaline detergent in hot tap water (approximately 50 °C)
- 50:50 isopropanol<sup>1</sup>/water
- 100% isopropanol<sup>1</sup>

Ideally, three beakers are prepared with each solvent, although the flushing steps in 50:50 isopropanol/water and isopropanol may be done consecutively in the same beaker.

The ultrasonic bath may be heated to 50 °C. Make sure to operate in a well-ventilated area and to cover the beakers with some aluminum foil or a watch glass when using isopropanol.

<sup>&</sup>lt;sup>1</sup> May be replaced by methanol or ethanol.

#### Purging

As the final step in each cleaning procedure, purge all ion optics parts with clean and oil-free nitrogen immediately after the last wipe with 100% isopropanol. Do not let solvents air-dry on the ion optics, especially water-containing ones. The part must be absolutely dry after the purging.

### **Frequency of Cleaning**

The frequency of cleaning the components of the API source 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 sample, the more rapidly it becomes dirty.

- The sample transfer line, the metal needle, and the API probe 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. See "Flushing the Sample Transfer Line, the Metal Needle, and the API Probe" on page 6-14.
- The ion transfer tube and the sweep cone of the API source must be removed and cleaned periodically. See "Removing, Cleaning, and Reinstalling the Ion Transfer Tube" on page 8-28.
- The S-lens and the ion funnel becomes dirty at a slower rate than the API probe, the sweep cone, and the ion transfer tube. See "Cleaning the S-lens/Ion Funnel" on page 8-40.

### **Removing and Reinstalling the API Source Housing**

You must remove the API source housing before you perform maintenance on the ion optics and the ion source interface.

This section contains the following topics:

- Removing the API Source Housing
- Installing the Ion Source Housing

#### **Removing the API Source Housing**

You must remove the API source housing to get access to the sweep cone.

### **CAUTION** Hot Parts. During operation of the mass spectrometer, the ion

transfer tube and the sweep cone can reach temperatures up to 450 °C. This might cause severe burns upon touching or ignite combustible material. The external surface of the ion source housing can reach temperatures up to 100 °C. This is hot enough to cause skin burns.

Do not touch the ion source housing when the mass spectrometer is in operation. Let the ion source cool down as described in this manual before you remove the ion source housing. Do not touch the ion source mount immediately after you have removed the ion source housing. Keep combustible materials away from the ion source mount. Do not let the instrument stay unattended when the housing is not mounted to the source.

**NOTICE** Dust can be sucked in through the ion inlet system. To reduce this risk to a minimum, keep an ion source housing installed on the mass spectrometer also during off times and standby times.

#### \* To remove the ion source housing

1. If the mass spectrometer was recently in operation, let the ion source housing cool down before you touch its external metal surface.

Set the tube temperature to 0 °C. Wait until the ion source has cooled down (approximately 30 minutes) before you do work on it.

- 2. If a probe is connected to the source housing, disconnect the external liquid lines before you remove the source housing from the mass spectrometer.
- 3. Rotate the ion source housing locking levers 90 degrees downwards to release the ion source housing from the ion source mount assembly.
- 4. Remove the ion source housing by pulling it straight off the ion source mount assembly. Place the housing in a safe location for temporary storage.

#### Installing the Ion Source Housing

#### To reinstall the ion source housing

1. Carefully align the two guide pin holes on the rear of the ion source housing (see Figure 8-9) with the ion source housing guide pins on

the mass spectrometer. Carefully press the ion source housing onto the ion source mount.





No.	Description	No.	Description
1	Locking lever (unlocked)	2	Guide holes on the back of the housing

 Rotate the ion source housing locking levers 90 degrees upwards to lock the ion source housing onto the ion source mount assembly. See Figure 8-10.

**Tip** Prevent solvent waste from backing up into the ion source and the mass spectrometer. Always make sure that liquid in the drain tube is able to drain to a waste container.

By default, the source gases will not drop below a minimum flow of 7 L/min to compensate for the suction through the transfer tube. This ensures a slightly positive pressure in the ion source to prevent solvent waste from being sucked back from the drain.



The ion source is now properly installed on the mass spectrometer.

Figure 8-10. OptaMax NG API source (front view)

No.	Description	No.	Description
1	Locking lever (locked position)	2	Window

#### **API Source Housing Maintenance**

User maintenance is limited to cleaning the API source housing as necessary. Follow all safety precautions in the sections regarding the installation and removal of the housing. For any additional service that might be necessary, contact your local Thermo Fisher Scientific field service engineer.

### **<u>CAUTION</u>**

**Hazardous Substance.** Methanol is highly flammable and noxious. Keep away from heat, sparks, and flame. Avoid accidental exposure. Use with adequate ventilation. When possible, dilute it with 50% water. Refer to your supplier's Material Safety Data Sheet (MSDS) for information about the correct handling of methanol.

#### \* To clean the API source housing

- 1. After the API source has cooled down to room temperature, remove it from the mass spectrometer.
- 2. Put on appropriate eye-wear and gloves.
- 3. Below an appropriate fume hood, rinse the interior of the housing with UHPLC/MS-grade methanol.

4. Allow the housing to dry before you install it on the mass spectrometer.

### Removing, Cleaning, and Reinstalling the Ion Transfer Tube

The bore of the ion transfer tube can become blocked by buffer salts or highly concentrated samples. The ion transfer tube can be removed for cleaning. You do not have to vent the system to remove the ion transfer tube.

If the pressure in the source region (as measured by the Pirani gauge) drops considerably below 1 mbar (2.5 mbar in case of an Orbitrap Exploris 480 MS), you should suspect a blocked ion transfer tube. You can check the Pirani gauge pressure in the Tune application.

# **WARNING** High Voltage. High voltages that can cause an electric shock are used in the instrument. Switch off the instrument before you proceed.

▲ CAUTION Hot Parts. During operation of the mass spectrometer, the ion transfer tube and the sweep cone might reach temperatures up to 450 °C. This might cause severe burns upon touching or ignite combustible material. The external surface of the ion source housing can reach temperatures up to 100 °C. This is hot enough to cause skin burns.

Do not touch the ion source housing when the mass spectrometer is in operation. Let the ion source cool down as described in this manual before you remove the ion source housing. Do not touch the ion source mount immediately after you have removed the ion source housing. Keep combustible materials away from the ion source mount. Do not let the instrument stay unattended when the housing is not mounted to the source.

#### **ACAUTION**

**Hazardous Substance.** Methanol is highly flammable and noxious. Keep away from heat, sparks, and flame. Avoid accidental exposure. Use with adequate ventilation. When possible, dilute it with 50% water. Refer to your supplier's Material Safety Data Sheet (MSDS) for information about the correct handling of methanol.

#### Maintenance of the Ion Transfer Tube and the Sweep Cone

The sweep cone of the Orbitrap Exploris 480 MS has a wider hole than the sweep cone of the other Orbitrap Exploris Series MSs. This difference is difficult to see unless both versions are placed side by side as shown in Figure 8-11. To avoid using the wrong sweep cone, the pins at the rear sides of the cones are positioned differently on both versions. When seen from behind, the sweep cone of Orbitrap Exploris 120, Orbitrap Exploris 240, and Orbitrap Exploris MX MS has the pin to the left of the sweep gas port. The sweep cone of Orbitrap Exploris 480 MS has the pin to the opposite side of the sweep gas port.





The Orbitrap Exploris 480 MS has a high capacity transfer tube with a rectangular orifice, where the larger aperture allows for a higher ion flux into the interface. The other Orbitrap Exploris Series MSs have a round bore ion transfer tube. The part numbers for the removal tools and the graphite seals are also different.



Orbitrap Exploris 120 MS Orbitrap Exploris 240 MS Orbitrap Exploris MX MS

Orbitrap Exploris 480 MS



See "Parts for Ion Source" on page 9-2 for a list of the parts that are necessary when you do maintenance of the ion transfer tube and the sweep cone. They are contained in the Installation Kit.

#### $\star$ To remove the ion transfer tube and the sweep cone

1. Switch off the flow of liquid from the LC (or an other sample introduction device) to the API source.

### NOTICE

2. In the Tune application window, place the system in Off mode. Wait for at least 60 minutes to let hot components cool down.

To prevent mechanical damage to the transfer tube, make sure that the tube temperature is well below 200 °C. Let the spray cone cool down for at least 60 minutes to allow safe handling by laboratory personnel. See the safety information on page 8-28.

- 3. Remove the API source housing from the front of the mass spectrometer as described on page 8-25.
- 4. Remove the sweep cone by grasping its outer ridges and pulling the cone straight off the API cone seal.

Do not accidentally lift the release lever (see Figure 8-13) at the top of the ion source interface, which will vent the MS.

To avoid contaminating the ion transfer tube, do not touch its exposed entrance.



**Figure 8-13.** Spray cone, O-ring, ion transfer tube, and sweep cone of the ion source interface (Orbitrap Exploris 120, Orbitrap Exploris 240, Orbitrap Exploris MX MS)

No.	Description	No.	Description
1	Release lever for the ion source interface	2	API cone seal
3	Spray cone	4	Vespel <sup>™</sup> O-ring
5	Ion transfer tube	6	Gas inlet on the sweep cone



- 5. Align the flat edges of the custom removal tool with the flat edges on the exposed tip of the ion transfer tube. Then do one of the following:
  - (Orbitrap Exploris 120, Orbitrap Exploris 240, Orbitrap Exploris MX MS) Rotate the tool (Figure 8-14) counterclockwise. When the tube is free of the spray cone, use the hook (flat edges) on the tool to pull it out of the ion source interface.



- **Figure 8-14.** Removing the ion transfer tube (Orbitrap Exploris 120, Orbitrap Exploris 240, Orbitrap Exploris MX MS)
  - (Orbitrap Exploris 480 MS) Using the correct end of the custom removal tool (Figure 8-15), rotate the ion transfer tube only 1/4-turn counterclockwise. Then, use the other end of the tool to remove the tube from the ion source interface.

**Tip** If necessary, insert a hex key through a side hole for leverage.



Use this end of the tool to hook onto and pull out the ion transfer tube.

Use this end of the tool to loosen and reinstall the ion transfer tube.





A protective mechanism prevents the air from entering the vacuum manifold. It requires that you drag the ion transfer tube with a quick and steady motion out of the spray cone.

#### \* To clean the ion transfer tube

- 1. Put the ion transfer tube in a beaker with a 2% solution of an alkaline detergent in water and sonicate for 30 minutes.
- 2. Remove the ion transfer tube from the beaker and rinse it thoroughly with a stream of tap water from all sides.
- 3. Sonicate the ion transfer tube in a 50:50 isopropanol/water solution for five minutes.
- 4. Sonicate the ion transfer tube in 100% isopropanol for five minutes.
- 5. Dry the ion transfer tube with a strong stream of oil-free nitrogen gas to make sure that the solvent evaporates completely.

#### \* To clean the sweep cone

- 1. Clean the inside and the outside of the sweep cone with lint-free wipes that have been soaked in a 50:50 isopropanol/water solution.
- 2. Clean the inside and the outside of the sweep cone with lint-free wipes that have been soaked in 100% isopropanol.
- 3. If the cone is still stained after the previous steps, use MICRO-MESH<sup>™</sup> 6000 to remove all stains and finish up with MICRO-MESH 12000.
- 4. Repeat steps 1 and 2.
- 5. Sonicate the cone in 100% isopropanol for five minutes.
- 6. Dry the cone with a strong stream of oil-free nitrogen gas to make sure that the solvent evaporates completely.

#### \* To clean the spray cone



Do not let any solvents get into the opening for the ion transfer tube as it might prevent the proper operation of the ball valve in the cage.

- 1. Clean the outside of the spray cone with lint-free wipes that have been soaked in a 50:50 isopropanol/water solution.
- 2. Clean the outside of the spray cone with lint-free wipes that have been soaked with 100% isopropanol.
- 3. If the cone is still stained after the previous steps, use MICRO-MESH<sup>™</sup> 6000 to remove all stains and finish up with MICRO-MESH 12000.
- 4. Repeat steps 1 and 2.

5. Dry the cone with a strong stream of oil-free nitrogen gas to make sure that the solvent evaporates completely.

#### ✤ To clean the O-ring in the spray cone

- 1. Remove and inspect the O-ring that is seated in the spray cone under the entrance end of the ion transfer tube. Clean it with methanol or replace it if necessary.
- 2. Reinsert the O-ring into the spray cone.

#### \* To reinstall the ion transfer tube and the sweep cone

- 1. Put on a new pair of lint- and powder-free gloves.
- 2. Insert the ion transfer tube into the heater block. Rotate the tube while you insert it.

NOTICE

When you reinstall the ion transfer tube into the heater block, take these precautions:

- Make sure that everything is properly aligned to prevent stripping the threads on the ion transfer tube.
- Do not bend the ion transfer tube.
- Insert the ion transfer tube with a quick and steady motion into the spray cone to prevent air from entering the vacuum manifold.
- 3. Align the gas inlet on the sweep cone with the sweep gas supply port on the ion source mount. Firmly press the sweep cone into the ion source mount.
- 4. Reinstall the API source housing on the mass spectrometer as described on page 8-25.
- 5. In the Tune application window, place the system in Standby condition.

If you have successfully cleared the ion transfer tube, then the Pirani gauge pressure should increase to a normal value (approximately 2 mbar [Orbitrap Exploris 120, Orbitrap Exploris 240, Orbitrap Exploris MX MS] resp. 3.5 mbar [Orbitrap Exploris 480 MS]). If you cannot clear the ion transfer tube by this method, then replace it.

### **API Probe Maintenance**

For the HESI probe, only minimum maintenance is necessary. If the metal needle is blocked, replace it. To replace the metal needle, you must partially disassemble the probe. Refer to the *OptaMax NG Ion Source User Guide* for instructions.

▲ **CAUTION** Hot Parts. At typical operating temperatures between 350 and 450 °C, touching the vaporizer might cause severe burns. Let the HESI probe cool to room temperature (approximately 60 minutes) before you touch or remove it.

For best results, do not operate the HESI probe at elevated temperatures without solvent flow. Letting the HESI probe to run dry at elevated temperatures can cause blockage of the replaceable metal needle.

**Tip** Wear a new pair of lint- and powder-free gloves when you handle HESI probe components. See "Personal Protective Equipment" on page 4-14 for a specification for the gloves.

#### Flushing the Sample Transfer Line and the Metal Needle

NOTICE

For best results, flush the sample transfer line, metal needle, and HESI probe for 15 minutes at the end of each working day (or more often if you suspect they are contaminated). Use a 50:50 methanol/distilled water solution from the LC system through the API source.

▲ CAUTION Hazardous Substance. Methanol is highly flammable and noxious. Keep away from heat, sparks, and flame. Avoid accidental exposure. Use with adequate ventilation. When possible, dilute it with 50% water. Refer to your supplier's Material Safety Data Sheet (MSDS) for information about the correct handling of methanol.

After 15 minutes, switch off the flow of liquid from the LC to the API source, but keep the API source on (including the sheath gas and auxiliary gas) for an additional 5 minutes. See "Flushing the Sample Transfer Line, the Metal Needle, and the API Probe" on page 6-14.

#### Ion Source Interface Maintenance

The ion source interface assembly includes the sweep cone, the ion transfer tube, the IC unit, and the S-lens/ion funnel. The ion transfer tube has a finite lifetime. You must replace it if its bore becomes corroded.

**Tip** The instructions in this section describe the maintenance for the Orbitrap Exploris 480 MS. If not indicated otherwise, the same instructions are also valid for the other Orbitrap Exploris Series MSs.

It is good practice to flush the sweep cone and the bore of the ion transfer tube at the end of each working day with a 50:50 methanol/water solution. See "Cleaning the Sweep Cone and the Ion Transfer Tube" on page 6-15.

For cleaning or replacement, you can remove the sweep cone and the ion transfer tube without venting the system. See "Removing, Cleaning, and Reinstalling the Ion Transfer Tube" on page 8-28.

#### **Sequence of Steps**

To maintain ion source interface assembly components other than the sweep cone and the ion transfer tube, proceed in this sequence:

Pro	cedure	Description
1.	Shut down and vent the system.	page 6-7
2.	Remove the API source housing.	page 8-25
3.	Remove the API source interface assembly.	page 8-36
4.	Clean the injection filter and the flatapole focus lens.	page 8-37
5.	Clean the IC unit and the S-lens or ion funnel.	page 8-40
6.	Reinstall the API source interface assembly.	page 8-42
7.	Reinstall the API source housing.	page 8-25
8.	Start up the system.	page 6-9

The above steps are described in the topics that follow.

#### **Removing the Ion Source Interface**

You must remove the ion source interface to access the IC unit and the S-lens/ion funnel.

### **A**CAUTION

**Hot Parts.** The ion source interface can become hot enough to cause severe burns when the mass spectrometer is in operation. Do not touch the ion source interface immediately after you have removed the ion source housing. Let the ion source interface cool until the temperature readback is <60 °C before you remove it from the mass spectrometer.

#### **\*** To remove the ion source interface

- 1. Shut down and vent the system as described on page 6-7.
- 2. Remove the ion source housing as described on page 8-25.
- 3. Put on a new pair of lint- and powder-free gloves. See page 4-14 for a recommendation for the gloves.
- 4. Lift up the release latch until it pushes the ion source interface out by a few millimeters.
- 5. Grasp the ion source interface with your fingers, and then carefully pull it out of the vacuum manifold (Figure 8-16).



Figure 8-16. Removing the ion source interface from the vacuum manifold

No.	Description	No.	Description
1	Release latch	2	Vacuum manifold

6. Place the assembly on a clean, lint-free surface.



Figure 8-17. Ion source interface (Orbitrap Exploris 480 MS)

No.	Description	No.	Description
1	Source cage	2	S-lens/Ion funnel
3	Internal calibration unit (see page 3-28)	4	Injection filter, with flatapole focus lens (not visible)

7. Block the opening to the analyzer chamber to prevent dust contamination, for example with the PEEK<sup>™</sup> accessory that comes with the instrument upon installation or a piece of aluminum foil.

#### **Cleaning the Injection Filter and the Flatapole Focus Lens**

#### \* To remove the injection filter

- 1. Put on a new pair of lint- and powder-free gloves. See page 4-14 for a recommendation for the gloves.
- 2. Insert a flat head screwdriver through the holes in the PEEK<sup>™</sup> holder of the injection filter. See Figure 8-18. Loosen the screws that attach the injection filter to the ion source interface cage. In this stage, the screws should turn freely and be movable by a few millimeters.
- 3. Remove the injection filter.
- 4. Put the components on a clean, lint-free surface.

See page 8-40 for instructions about cleaning the ion funnel/S-lens and page 8-20 for instructions about cleaning the IC unit.



Figure 8-18. Removing the injection filter

#### \* To remove the flatapole focus lens

- 1. Pull up on the top tab of the metal retainer for the flatapole focus lens until it is freed from the PEEK holder.
- 2. Unhook the bottom side of the retainer and remove the lens. Clean the body of the injection filter as described on page 8-37.
- 3. Remove the O-ring (see Figure 8-19).





No.	Description	No.	Description
1	O-ring	2	Injection filter
3	Flatapole focus lens	4	Retainer

#### \* To clean the injection filter

- 1. Sonicate the injection filter in a 2% solution of an alkaline detergent in water for 5 minutes.
- 2. Remove the injection filter from the beaker.
- Clean the rod surfaces facing the ion beam with a lint-free swab that has been soaked in a 2% solution of an alkaline detergent in water. Wipe each rod 20 times (apply gentle pressure to the swab handle). Turn the injection filter around and repeat from the other side.
- 4. Sonicate the injection filter in a 2% solution of an alkaline detergent in water for 10 minutes.
- 5. Rinse the component thoroughly with warm tap water.
- 6. Sonicate the component in a 50:50 isopropanol/water solution for five minutes.
- 7. Sonicate the component in 100% isopropanol for five minutes.
- 8. Dry the component with a strong stream of oil-free nitrogen gas to make sure that the solvent evaporates completely.
- 9. With a magnifying device, inspect the component for any lint, particulates, and sample buildup or coatings. Use plastic tweezers or a similar tool to remove lint or particulates.

#### \* To clean the flatapole focus lens

- 1. Clean the inside of the orifice with a conical swab that has been soaked in a 50:50 isopropanol/water solution.
- 2. Clean the lens orifice from both sides with a lint-free wipe that has been soaked in a 50:50 isopropanol/water solution.
- 3. Clean the lens orifice from both sides with a lint-free wipe that has been soaked in 100% isopropanol.
- 4. Dry the component with a strong stream of oil-free nitrogen gas to make sure that the solvent evaporates completely.

#### \* To reinstall the flatapole focus lens

- 1. Reinstall the O-ring onto the lens.
- 2. Place the flatapole focus lens onto the injection filter assembly. Then hook the lower part of the holder clip under the holder. Slide it with both thumbs from the bottom to the top, so that it clips onto the top.

#### ✤ To reinstall the injection filter

With a flat head screwdriver, attach the injection filter back to the ion source interface cage with the screws. Use the pin for alignment.

#### **Cleaning the S-lens/lon Funnel**

Remove the ion funnel and the IC unit from the ion source interface cage before you clean them.



Figure 8-20. Exploded view of the ion source interface cage (Orbitrap Exploris 480 MS)

No.	Description	No.	Description
1	Ion funnel	2	IC unit
3	Thumbscrews	4	Lead pin socket
5	Ion funnel holder	6	Ion source interface cage

#### \* To remove the S-lens/ion funnel from the ion source interface cage

- 1. Cover the area with lint-free paper or aluminum foil to prepare a clean work surface.
- 2. Put on a new pair of lint- and powder-free gloves. See page 4-14 for a recommendation for the gloves.
- 3. Loosen and extend the two thumbscrews that secure the S-lens/ion funnel to the ion source interface cage and the IC unit to the S-lens/ion funnel .
- 4. Grasp the two thumbscrews and carefully pull the S-lens/S-lens/ion funnel straight out of the ion source interface cage. Place it on a clean, lint-free surface.

- 5. With the thumbscrews extended, continue turning them counterclockwise until they are only holding in the IC unit/reagent ion source assembly.
- 6. Pull on the two thumbscrews again to separate the IC unit /reagent ion source from the S-lens/ion funnel.
- 7. Put the IC unit on a clean, lint-free surface.
- \* To clean the ion funnel or the S-lens/ion funnel

NOTICE

Do not clean the lenses with abrasives, acidic or caustic substances, or detergents that are not stated in this manual. Do not disassemble the S-lens/ion funnel from its holder. Otherwise, you risk losing the correct alignment of the lens segments.

- 1. Put on a new pair of lint- and powder-free gloves. See page 4-14 for a recommendation for the gloves.
- Put the S-lens/ion funnel in a beaker with a 2% solution of an alkaline detergent in water with the PEEK holder facing down. Up to 10% alkaline detergent can be used in case of an extreme contamination.
- 3. Sonicate the S-lens/ion funnel for 60 minutes.
- 4. Additional step for Orbitrap Exploris 120, Orbitrap Exploris 240, and Orbitrap Exploris MX MSs: Clean the S-lens/ion funnel with chamois-tipped swabs that have been soaked in a 2% solution of an alkaline (or neutral) detergent in water. To clean the areas that you cannot reach with the swab, use 6000 grit MICRO-MESH polishing swabs.
- 5. Rinse the S-lens/ion funnel thoroughly with warm, running tap water.
- 6. Sonicate the S-lens/ion funnel in deionized water for five minutes.
- 7. If you used a high concentration of detergent in step 2, then repeat the steps 5 and 6 five times with fresh water.
- 8. Sonicate the S-lens/ion funnel in a 50:50 isopropanol/water solution for five minutes. If noticeable residues come off the S-lens/ion funnel in this stage, then repeat the steps 2 to 8 until this is not noticeable anymore.
- 9. Sonicate the S-lens/ion funnel in 100% isopropanol for five minutes.
- 10. Dry all components with a strong stream of oil-free nitrogen gas to make sure that the solvent evaporates completely. Start with purging all drill holes and narrow gaps.

11. With a magnifying device, inspect the components for any lint, particulates, and sample buildup or coatings.

#### \* To clean the IC unit

Follow the instructions on page 8-20.

#### \* To reinstall the S-lens/ion funnel

- 1. Put on a new pair of lint- and powder-free gloves. See page 4-14 for a recommendation for the gloves.
- 2. Align the lead pin on the IC unit with the lead pin socket on the S-lens/ion funnel (see Figure 8-20 on page 8-40)<sup>4</sup>, and then firmly press the unit until it snaps into place.
- 3. Tighten the two thumbscrews a few turns into the S-lens/ion funnel.
- 4. Orient the S-lens/ion funnel as shown in Figure 8-20, and then carefully slide it into the ion source interface cage.
- 5. Tighten the two thumbscrews a few turns into the ion source interface cage.

Continue with "Reinstalling the Ion Source Interface."

#### **Reinstalling the Ion Source Interface**

Before you install the ion source interface, inspect the O-ring for damage. Replace it if necessary.

#### \* To reinstall the ion source interface

- 1. Orient the ion source interface with the release latch at the top (see Figure 8-16 on page 8-36).
- 2. Carefully insert the ion source interface into the vacuum manifold. Push until there is no or only a small gap left between the two.
- 3. Reinstall the ion transfer tube and lock it with a quarter turn. See page 8-33.
- 4. Reinstall the ion source housing as described on page 8-25.

If necessary, reinstall the ion source probe and the LC liquid lines.

- 5. Start up the system as described on page 6-9.
- 6. Run the Ion Optics Connectivity Check from the Diagnostics pane in the Tune application.

Now you can start using the instrument again.

### **Maintaining LCs or Autosamplers**

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

### Consumables

For information on consumables such as fittings, nitrogen gas, or cleaning agents, refer to the *Orbitrap Exploris Series Pre-Installation Requirements Guide*, chapter *Consumables*.

For information on calibration- and test-chemicals or solvents, see "Obtaining the Calibration Solution" on page 5-30.

The forepump oil is used for the cooling, the lubrication, and the sealing of the forepump. See page 9-3 for the specification of the forepump oil. See "Maintenance of the Forepumps" on page 8-10 for information about forepump oil disposal. Also refer to the Material Safety Data Sheet (MSDS) for the forepump oil.

See also "Permitted Materials" on page 4-6 for information about personnel safety.

### **Thermo Fisher Scientific Service**

This section contains information concerning maintenance work that must be performed by Thermo Fisher Scientific personnel.

### **Returning Parts**



**Hazardous Chemicals.** Hazardous material might contaminate certain parts of your system during analysis. To protect our employees, we ask you to adhere to special precautions when you send back parts to the factory for exchange or repair.

If hazardous materials have contaminated instrument parts, Thermo Fisher Scientific can only accept these parts for repair if they have been properly decontaminated.

Materials that might be toxic due to their structure and the applied concentration or that are reported in publications to be toxic are regarded as hazardous. Materials that will cause synergetic hazardous effects in combination with other materials present are also considered hazardous.

Parts that are contaminated by radioisotopes must not be returned to Thermo Fisher Scientific—neither under warranty nor within the exchange part program. If you are unsure whether parts of the system are possibly contaminated by hazardous material, make sure that the Thermo Fisher Scientific field service engineer is informed before the engineer starts to do work on the system.

Your signature on the Health and Safety Form confirms that the returned parts have been decontaminated and that they are free of hazardous materials. You can download this form from the SharePoint (see page 1-5). Instead, request a copy from the Thermo Fisher Scientific field service engineer.

### Services to be Performed by Thermo Fisher Scientific Service Only

Table 8-4 lists services that must be performed only by a Thermo Fisher Scientific field service engineer. Depending on the actual workload of your Orbitrap Exploris Series mass spectrometer, you might increase the maintenance frequency.

#### Table 8-4. Thermo Fisher Scientific service procedures

MS Component	Procedure	Frequency
ТМР	Change operating fluid reservoir	Every four years
	Change TMP bearing	Every four years

## **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 Orbitrap Exploris Series system, order only the parts listed or their equivalent.

For information on how to order parts, see "Contacting Us" on page 1-5.

#### Contents

- Ion Source Probes and Parts on page 9-2
- Instrument Parts on page 9-3

### Ion Source Probes and Parts

Refer also to the *OptaMax NG Ion Source User Guide* for more lists of replaceable parts for the OptaMax NG API source and available API probes. See also "Obtaining the Calibration Solution" on page 5-30.

APCI Probe Kit	. OPTON-32101
APPI Probe Kit	. OPTON-30350

### **Parts for Ion Source**

ESI Calibration spray probe with low flow needle	OPTON-20065
Low flow HESI needle	OPTON-30139
Tool, probe capillary length	80000-20957

# Orbitrap Exploris 120 MS, Orbitrap Exploris 240 MS, Orbitrap Exploris MX

Sweep cone	80111-20646
Ion transfer tube	70005-20606
Ion transfer tube removal tool	70111-20258
Graphite Vespel <sup>™</sup> seal ring	97055-20442

#### **Orbitrap Exploris 480 MS**

80100-20646
80500-20045
70005-20972
70005-20922

#### **Source Accessory Parts**

Syringe 500 μL	 
Syringe Adaptor Kit	 

#### **Source Drain Parts**

Tubing, Tygon<sup>m</sup>, 1-3/8 in. OD, 1 in. ID, 3 m (10 ft) .....00301-01-00020 Spiral coiled tube, PVC, ID=25 mm, OD=31 mm ..... BRE0011767 Container, Nalgene<sup>m</sup>, 4 L heavy-duty; filling/venting cap ..... 80100-20265
## **Instrument Parts**

#### **Gas Supply Parts**

Teflon hose	, OD 6 mm /	ID 4 mm	
-------------	-------------	---------	--

#### **Forevacuum Parts**

#### **Ethernet Switch and Cables**

Switch	2108640
Patch cord, RJ45 SFTP, 5 m	2125930
Patch cord, RJ45 SFTP, 1m	2125920

#### Plug Connectors (to connect other devices of the LC/MS system)

COMBICON_MC1.5/8ST-3.81	2087270
KGG MC1.5/8 cable housing	2087280

#### **Additional Hardware**

Syringe pump Chemyx SKE10	BRE0011389
Divert/inject valve, Rheodyne MX Series II	

Replaceable Parts Instrument Parts

9-4 Orbitrap Exploris Series Operating Manual (P/N BRE0014471, Revision E)

## **Legal Documents**

#### Contents

- FCC Compliance Statement on page A-2
- WEEE Compliance on page A-3
- EU REACH Statement on page A-4
- EU Declaration of Conformity on page A-5
- UK Declaration of Conformity on page A-6

## **FCC Compliance Statement**

This equipment has been tested and found to comply with the limits for a Class B digital device, pursuant to Part 15 of the FCC Rules. These limits are designed to provide reasonable protection against harmful interference in a residential installation. This equipment generates, uses and can radiate radio frequency energy and, if not installed and used in accordance with the instructions, may cause harmful interference to radio communications. However, there is no guarantee that interference will not occur in a particular installation. If this equipment does cause harmful interference to radio or television reception, which can be determined by turning the equipment off and on, the user is encouraged to try to correct the interference by one or more of the following measures:

- Reorient or relocate the receiving antenna.
- Increase the separation between the equipment and receiver.
- Connect the receiver into an outlet on a circuit different from that to which the equipment is connected.
- Consult the dealer or an experienced radio/TV technician for help.

## **WEEE Compliance**

This product is required to comply with the European Union's Waste Electrical & Electronic Equipment (WEEE) Directive 2012/19/EU. It is marked with the following symbol:



Thermo Fisher Scientific is registered with B2B Compliance (B2Bcompliance.org.uk) in the UK and with the European Recycling Platform (ERP-recycling.org) in all other countries of the European Union and in Norway.

If this product is located in Europe and you want to participate in the Thermo Fisher Scientific Business-to-Business (B2B) Recycling Program, send an email request to weee.recycle@thermofisher.com with the following information:

- WEEE product class
- Name of the manufacturer or distributor (where you purchased the product)
- Number of product pieces, and the estimated total weight and volume
- Pick-up address and contact person (include contact information)
- Appropriate pick-up time
- Declaration of decontamination, stating that all hazardous fluids or material have been removed from the product



This recycling program is not for biological hazard products or for products that have been medically contaminated. You must treat these types of products as biohazard waste and dispose of them in accordance with your local regulations.

## **EU REACH Statement**

The European Commission promulgated legislation that covers the registration, evaluation, authorization and restriction of chemicals within the European Union community under (EC) No 1907/2006. This regulation is commonly known as REACH. Thermo Fisher Scientific is committed to meeting all compliance obligations under REACH. As per Article 33 of the Regulation, this product may include items which contain more than 0.1% by weight of some SVHC Candidate Substance. Some electronic parts and copper alloys can contain lead.

## **EU Declaration of Conformity**

-Original-

## **EU-Konformitätserklärung** *EU Declaration of Conformity*

CE



Thermo Fisher Scientific (Bremen) GmbH Hanna-Kunath-Str. 11 28199 Bremen, Germany

Wir erklären hiermit, dass die folgenden Produkte We hereby declare that the following products

Bezeichnung: Designation: Massenspektrometer Mass Spectrometer

Modell: Model: Thermo Scientific Orbitrap Exploris Serie Thermo Scientific Orbitrap Exploris Series (Orbitrap Exploris 120, Orbitrap Exploris 240, Orbitrap Exploris 480, Orbitrap Exploris MX)

alle einschlägigen Anforderungen der folgenden Richtlinien erfüllen: fulfill all the relevant requirements of the following directives:

Niederspannungsrichtlinie Low Voltage Directive

Richtlinie über elektromagnetische Verträglichkeit Electromagnetic Compatibility Directive **2014/30/EU** 2014/30/EU

2014/35/EU

2014/35/EU

**Die folgenden einschlägigen harmonisierten Normen wurden zugrunde gelegt:** *The following relevant harmonized standards were used:* 

EN 61010-1:2010/A1:2019 EN 61010-1:2010/A1:2019 EN 61326-1:2013 EN 61326-1:2013

**Für die Zusammenstellung der technischen Unterlagen ist bevollmächtigt:** *Person authorized to compile the technical file:* 

Rainer Bröring (Geschäftsführer) Thermo Fisher Scientific (Bremen) GmbH

Unterschrift

Unterschrift Signature Bremen, July-28, 2021

Datum Date

## **UK Declaration of Conformity**

-Original-

## **UK Declaration of Conformity**





Thermo Fisher Scientific (Bremen) GmbH Hanna-Kunath-Str. 11 28199 Bremen, Germany

Declares, under sole responsibility, that products

**Designation:** 

**Mass Spectrometer** 

Model:

Thermo Scientific Orbitrap Exploris Series (Orbitrap Exploris 120, Orbitrap Exploris 240, Orbitrap Exploris 480, Orbitrap Exploris MX)

as originally delivered complies with the essential requirements of the following applicable UK Regulations:

Electrical Equipment (Safety) Regulations	2016
Electromagnetic Compatibility Regulations	2016
The Restriction of the Use of Certain	2012

Hazardous Substances in Electrical and Electronic Equipment (ROHS) Regulations

and complies with the following harmonized standards and other technical specifications:

BS EN 61010-1:2010

BS EN 61326-1:2013

Signed for and on behalf of: Thermo Fisher Scientific (Bremen) GmbH:

Rainer Bröring (Geschäftsführer) Thermo Fisher Scientific (Bremen) GmbH

Signature

Bremen, 2021-05-08

## **Component Suppliers' Documents**

This appendix contains excerpts from component suppliers' documents with safety-relevant information that may concern users of Orbitrap Exploris Series mass spectrometers.

#### Contents

- Forepumps on page B-2
- Syringe Pump on page B-4

## Forepumps

Observe the following safety guidelines when you operate the forepump.

## **SOGEVAC Pumps**

Failure to observe the following precautions could result in serious personal injury!

SOGEVAC<sup>™</sup> pumps are not designed:

- for pumping of dusty, aggressive, corrosive, flammable or explosive gases or gas mixtures,
- for pumping of oxygen or other highly reactive gases with a greater concentration than atmospheric concentration (>20%),
- for working in flammable, explosive or dusty environment.

For all these cases, special materials must be used. In case of doubt, contact Oerlikon Leybold Vacuum. See also the limits of use indicated in the CE declaration of conformity.

**WARNING** High Voltage. When you touch parts at high electric voltages, there is the risk that you suffer severe injuries by an electric shock! Covers marked with this symbol must be opened only by trained electricians after having reliably deenergized (lockout/tagout) the equipment.

Always operate the pump with a properly connected grounding conductor and make sure that the motor & FC connection box are closed.

- **WARNING** High Voltage. Even if the pump is not operating, there is the risk of suffering severe injuries by an electric shock! Even after complete power disconnection, live voltage is present in the frequency converter. Wait a minimum of 10 minutes for a complete capacitor discharge.
- **Explosion Hazard.** The standard pump is not suitable for installation in explosion hazard ATEX areas. Contact the pump manufacturer if you are planning such an application. Before you install the pump, you must reliably disconnect it from the electrical power supply and prevent the pump form running up inadvertently.
- **CAUTION Tripping Hazard.** Lay electric feed lines so that there is no risk of tripping over these.

<b>ACAUTION</b>	<b>Hot Parts.</b> In normal operation, the pump surface temperature can reach 85 °C. Touching parts of the forepump might cause burns. Switch off the pump and let it cool down before any intervention or take appropriate precautions. It is recommended to use an oil casing or pump touching protection at high ambient temperatures.
	As a protection against touching, you can use the noise reduction cover.
	Always wear heat protective gloves when you work on a pump that is "still warm from operation."
	Handle the pump only when it is vented and after having let it cool down.
	Do not remove the oil-fill or oil-drain plugs while the pump is running. There exists the risk of suffering burns. Always wear protective gloves and protective goggles also for protection against the oil.
	Vacuum Hazard. Risk of injury. Do not expose part of the body to the vacuum.
	Do not operate the pump with an open and thus accessible inlet. Vacuum connections as well as oil filling and oil draining openings must not be opened during operation of the pump.
	Depending on the process involved, dangerous substances and oil might escape from the pump. Take the necessary safety precautions!
	Disconnect the unit from the power supply before starting any work.
<b>WARNING</b>	<b>Toxic Vapors</b> Risk of poisoning when igniting and heating synthetic operating fluids (e.g. F4/F5) above 300 °C. Observe the application instructions of the operating fluid manufacturer. Do not allow operating fluid to make contact with tobacco products. Observe safety precautions when you handle chemicals.
	Steens Manual Field in the Wisin its of the Daine Sectors I Long
<b>VVARNING</b>	to life for persons with cardiac pacemakers when the drive system Hazard disassembled. Persons with cardiac pacemakers must not enter the area of the magnetic field. Disassembled magnetic couplings must be kept away from computers, data storage media and other electronic components.

**DUO Pump** 

<b><u>CAUTION</u></b>	<b>Emission of Toxic Substances from the Exhaust</b> Risk of poisoning from emitted gases or vapors, which can be detrimental to health and/or can pollute the environment, depending on the particular application. Comply with the applicable regulations when working with toxic substances. Only officially approved filter systems may be used to separate out these substances.
<b><u>CAUTION</u></b>	<b>Risk of Injury from Moving Parts</b> After power failure or motor shutdown due to overheating, the motor may restart automatically. Secure the motor so that it cannot be switched on while any work is being performed on the pump. If necessary, dismantle the pump from the installation for inspection.
<b>CAUTION</b>	<b>Hot Surface</b> Risk of burns if hot parts are touched. Depending on the operating and ambient conditions, the surface temperature of the pump may rise above 70 °C. In this case, use suitable finger guards. The surface temperature of the pump may rise above 105 °C in case of malfunction. Carry out work on the pump only after it has cooled to a safe temperature
<b>CAUTION</b>	<b>Pump Parts may be Contaminated from Pumped Media</b> Risk of poisoning due to contact with harmful substances. Decontaminate the pump before carrying out any maintenance work. In the event of contamination, take suitable safety precautions to prevent your health from being harmed by any dangerous substances.
<b>CAUTION</b>	Hot Operating Fluid Risk of burns when draining due to contact with skin. Wear suitable protective clothing.
<b><u>CAUTION</u></b>	<b>Operating Fluid may contain Toxic Substances from the Pumped</b> <b>Media</b> Danger of poisoning from the emission of harmful substances (radioactive, toxic, etc.) from the operating fluid. Wear suitable protective clothing and respirators. Dispose of operating fluid according to the local regulations.
Syringe Pump	Observe the following safety guidelines when you operate the syringe
	pump.
	<b>Pinch Hazard</b> . Do not place fingers between the pusher block and end block while the pump is running.

# C

## **Accessing the Technical Documentation SharePoint**

Use the Technical Documentation SharePoint to download current revisions of user manuals and other customer-facing documents for your product. Translations into other languages may be available as well. The SharePoint also provides access to videos and software.

#### Contents

- Creating a User Account on page C-1
- Accessing the SharePoint for the First Time on page C-3
- Accessing the SharePoint as registered Customer on page C-4
- Using the SharePoint on page C-5
- Receiving Update Messages on page C-6

## **Creating a User Account**

#### To create a user account

1. Click www.thermofisher.com/Technicaldocumentation or enter that address manually.

Your Internet browser displays a Start page.

SCIENTIFIC	
Technical Documentation Bremen For customers:	For Thermo Fisher Scientific employees:
Login >	Login >
Only for the first login: <u>Create an account</u>	Login with your Thermo Fisher credentials
y submitting your data, you agree to our <u>Privacy Policy</u> .	ThermoFishe

Figure C-1. Start page

2. Click Create an account.

Your Internet browser displays a page with a short guide.

Creating a User Account

Create an Account for th	ie First Log-In
Step 1: Fill out the acce Step 2: After you compl	es request form ated Step 1, you will receive an invitation email from Microsoft-SharePoint, within 24 hours. Please, click on "Go To Technic
Documentation Bremen	
	Office 365
Hello,	

#### Figure C-2. Guide

3. Click the link in Step 1 of the guide to display the access request form.

Your Internet browser displays the access request form.

Technical Documentation Please fill in the form to n Your request will be sent	1 Bremen request access the Technical Docu to our technical documentation gr	mentation Bremen system.
		oup. You will soon receive an email with log in information.
irst Name: *		Instrument Group: * - Select Instrument Group 🗸
ast Name: *		LSMS: Exactive-, LTQ FT- and LTQ Orbitrap Series
Company: *		Gas IRMS Instruments: Delta Series, Breath MAT Plus, MAT
Country: *	- Please select	Gas IRMS Periphals: ConFlo, Dual Inlet, Element Analyzers, Cos Dande CC, CC (Colleging & Davido, Kiel IV Corbergia
Email Address: *		Device, LC IsoLink, p-Volumn
		Service Number: (begins with SN)*
		Submit Form

Figure C-3. Access request form

4. Enter the requested data in the appropriate fields. Select the requested entries in the list boxes for Country and Instrument Group.

All entries are mandatory. Provide the email address that you use in your company or institution. Do not provide any private email addresses.

**Tip** This form requests for a Service Number. Please use the **Serial** Number instead. The Serial Number of your instrument is given on the name plate attached to your instrument. Refer to the Operating Manual for the location.

5. When you are finished, click **Submit Form** to send your data to Thermo Fisher Scientific.

Thermo Fisher Scientific will check your data to make sure that you are a legitimate customer. When the check is successful, you will receive an invitation to the SharePoint. Now, you have six days to log into the SharePoint with your Microsoft<sup>™</sup> password.

## Accessing the SharePoint for the First Time

The SharePoint requires that you have a Microsoft account for the email address that you use in your company or institution. If you have not already done so, create a Microsoft account by following the instructions on the Microsoft website.

**Tip** If your computer runs with Windows 10, you have most likely set up a Microsoft account during the installation.

- ✤ To access the SharePoint for the first time
- 1. On the invitation email from the Microsoft SharePoint, click **Go To Technical Documentation Bremen**.



Figure C-4. Invitation email

2. On the Welcome page, click Create a Microsoft SharePoint Online account.



Figure C-5. Welcome page

Accessing the SharePoint as registered Customer

3. Click Microsoft account.



Figure C-6. Choosing Microsoft account

4. Log in with your Microsoft credentials. Enter the email address and the password.



Figure C-7. Signing in

5. Click Sign In.

## Accessing the SharePoint as registered Customer

#### \* To access the SharePoint as a registered customer

1. Click www.thermofisher.com/Technicaldocumentation or enter that address manually.

On the Start page, click the **Login** button on the **left** side.

Thermo SCIENTIFIC		
Technical Documentation Bremen For customers:	For Thermo Fisher Scientific employees:  Login Login with your Thermo Fisher credentials	
By submitting your data, you agree to our <u>Privacy Policy</u> . © Thermo Fisher Scientific Inc. All rights reserved.		ThermoFisher SCIENTIFIC

Figure C-8. Customer login

2. On the Login page, click Technical Documentation Bremen Site.



Figure C-9. Login page

3. Your Internet browser displays the Start page of the Technical Documentation SharePoint.

You have access to documents that are relevant for the instrument that you have registered at "Creating a User Account" on page C-1 and to documents that are relevant for all users. The figure shows the Start page for a user who has registered a multicollector ICP-MS (a Neptune MS, for example).



Figure C-10. Start page of the Technical Documentation SharePoint

## **Using the SharePoint**

On the SharePoint, you can use either the links on the Navigation pane on the left or the links on the Content pane on the right.

If an instrument group contains several instruments, click the tiles to go to the page of your instrument.

Receiving Update Messages



Figure C-11. Instrument Group page

On an instrument page, the available documents are displayed in tables. Click the title of a column to sort the entries or to apply a filter. If more than five documents are available for your instrument, a scroll button appears at the bottom of the table. To download a document, right-click the entry under Name and choose **Save Link as**.

English Documents					
	Document type	Title	Information	Туре	Name
	Others			pdf	1250910_Jet_Interface_User_Guide_Rev_A
	Others	High-Resolution Peak center		<u>edf</u>	1378220_HighResolutionPeakCenter_Manual_Rev_A
	Others	UK Declaration of Conformity		pdf	2020_DoC_UK_Neptune Series
	Operating Manual	GCI 300 Transfer Line Operating Manual		<u>edf</u>	BRE0006945_GCI 300_Operating Manual_RevD
	Operating Manual	Neptune Series Operating Manual	1250710, Rev. G	pdf	NeptuneSeries_OM
			4 6-10 ▶		

Figure C-12. Available documents

## **Receiving Update Messages**

You can configure the SharePoint to notify you when a page was updated.

#### ✤ To activate the alerts for a SharePoint page

- 1. Browse to the page that you want to have alerts for.
- 2. Click the Page tab in the top left corner to display the toolbar.

#### Accessing the Technical Documentation SharePoint

Receiving Update Messages



Figure C-13. Page tab

3. Click the Alert Me button to display the menu.



Figure C-14. Alert Me button

- 4. Choose Set an alert on this page.
- 5. On the alert settings dialog box, make the required changes. We recommend that you select a daily summary of the changes.

#### Accessing the Technical Documentation SharePoint

Receiving Update Messages

с т	Site Pages: 253 Plus.aspx - New Alert				
n (, 2	Alert Title         Site Pages: 253 Plus.aspx         Ca           Enter the title for this alert. This is included in the subject of the notification sent for this alert.         Site Pages: 253 Plus.aspx         Site Pages: 253 Plus.aspx				
ie. IS	Delivery Method Specify how you want the alerts delivered.	Send me alerts by:			
חג -	Send Alerts for These Changes Specify whether to filter alerts based on specific criteria. You may also restrict your alerts to only include items that show in a particular view.	Send me an alert when: Anything changes Someone else changes a wiki page Someone else changes a wiki page created by me Someone else changes a wiki page last modified by me Someone changes an item that appears in the following view: Created By Me			
>n =nf he ou /la	When to Send Alerts Specify how frequently you want to be alerted. (mobile alert is only available for immediately send)	<ul> <li>Send notification immediately</li> <li>Send a daily summary</li> <li>Send a weekly summary</li> <li>Time:</li> <li>Wednesday</li> <li>4:00 AM</li> </ul>			
		OK Cancel			

Figure C-15. Alert settings dialog box

- 6. Click **OK** to save your changes and close the dialog box.
- 7. Depending on your settings, an email message or SMS message will confirm that you have activated the alert.

From now on, you will be notified when the page is updated.

## Glossary

This section lists and defines terms used in this manual. It also includes acronyms, metric prefixes, symbols, and abbreviations.

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

#### A

A ampere

AC alternating current

- **ADC** analog-to-digital converter; a device that converts data from analog to digital form.
- **adduct ion** An ion formed by the joining together of two species, usually an ion and a molecule, and often in the ion source, to form an ion containing all the constituent atoms of both species.
- **AGC<sup>™</sup>** See Automatic Gain Control<sup>™</sup> (AGC).
- **All Ion Fragmentation (AIF)** Acquisition mode that applies an HCD fragmentation to all ionized molecules without mass filtering.

See also Higher energy Collision-induced Dissociation (HCD).

**APCI** See atmospheric pressure chemical ionization (APCI).

**APCI corona discharge current** The ion current carried by the charged particles in the APCI source. The voltage on the APCI corona discharge needle supplies the potential required to ionize the particles. The APCI corona discharge current is set; the APCI corona discharge voltage varies, as required, to maintain the set discharge current.

See also corona discharge and APCI corona discharge voltage.

**APCI corona discharge voltage** The high voltage that is applied to the corona discharge needle in the APCI source to produce the APCI corona discharge. The corona discharge voltage varies, as required, to maintain the set APCI spray current.

See also APCI spray current.

- **APCI manifold** The manifold that houses the APCI sample tube and nozzle, and contains the plumbing for the sheath and auxiliary gas.
- **APCI needle, corona discharge** A needle to which a sufficiently high voltage (typically ±3 to ±5 kV) is applied to produce a chemical ionization plasma by the corona discharge mechanism.

See also chemical ionization (CI), chemical ionization (CI) plasma, atmospheric pressure chemical ionization (APCI), and corona discharge.

**APCI nozzle** The nozzle in the APCI probe that sprays the sample solution into a fine mist.

See also atmospheric pressure chemical ionization (APCI).

**APCI sample tube** A fused silica tube that delivers sample solution to the APCI nozzle. The APCI sample tube extends from the sample inlet to the APCI nozzle.

See also atmospheric pressure chemical ionization (APCI), and API stack.

**APCI source** Contains the APCI probe assembly, APCI manifold, and API stack.

See also atmospheric pressure chemical ionization (APCI), APCI manifold, and API stack.

- **APCI spray current** The ion current carried by the charged particles in the APCI source. The APCI corona discharge voltage varies, as required, to maintain the set spray current.
- **APCI vaporizer** A heated tube that vaporizes the sample solution as the solution exits the sample tube and enters the atmospheric pressure region of the APCI source.

See also atmospheric pressure chemical ionization (APCI).

API See atmospheric pressure ionization (API).

- **API atmospheric pressure region** The first of two chambers in the API source. Also referred to as the spray chamber.
- **API capillary-skimmer region** The area between the capillary and the skimmer, which is surrounded by the tube lens. It is also the area of first-stage evacuation in the API source.
- **API ion transfer tube** A tube assembly that assists in desolvating ions that are produced by the ESI, NSI, or APCI probe.

See also API ion transfer tube offset voltage and API ion transfer tube temperature.

**API ion transfer tube offset voltage** A DC voltage applied to the ion transfer tube. The voltage is positive for positive ions and negative for negative ions.

See also API source and API ion transfer tube.

**API ion transfer tube temperature** The temperature of the ion transfer tube, which should be adjusted for different flow rates.

See also API source and API ion transfer tube.

**API source** The sample interface between the LC and the mass spectrometer. It consists of the API probe (ESI or APCI) and API stack.

See also atmospheric pressure ionization (API), ESI source, APCI source, ESI probe, and API stack.

**API spray chamber** The first of two chambers in the API source. In this chamber the sample liquid exits the probe and is sprayed into a fine mist (ESI or NSI) or is vaporized (APCI) as it is transported to the entrance end of the ion transfer tube.

**API spray shield** A stainless steel, cylindrical vessel that, in combination with the ESI or APCI flange, forms the atmospheric pressure region of the API source.

See also atmospheric pressure ionization (API).

**API stack** Consists of the components of the API source that are held under vacuum and includes the API spray shield, API ion transfer tube, API tube lens, skimmer, the ion transfer tube mount, and the tube lens and skimmer mount.

See also atmospheric pressure ionization (API) and API source.

**API tube lens** A lens in the API source that separates ions from neutral particles as they leave the ion transfer tube. A potential applied to the tube lens focuses the ions toward the opening of the skimmer and helps to dissociate adduct ions.

See also API tube lens offset voltage, API source, API ion transfer tube, and adduct ion.

- **API tube lens and skimmer mount** A mount that attaches to the heated capillary mount. The tube lens and skimmer attach to the tube lens and skimmer mount.
- **API tube lens offset voltage** A DC voltage applied to the tube lens. The value is normally tuned for a specific compound.

See also API tube lens, adduct ion, and source CID.

**AP-MALDI** See atmospheric pressure matrix-assisted laser desorption/ionization (AP-MALDI).

**APPI** See Atmospheric Pressure Photoionization (APPI).

- **ASCII** American Standard Code for Information Interchange
- **atmospheric pressure chemical ionization (APCI)** A soft ionization technique done in an ion source operating at atmospheric pressure. Electrons from a corona discharge initiate the process by ionizing the mobile phase vapor molecules. A reagent gas forms, which efficiently produces positive and negative ions of the analyte through a complex series of chemical reactions.

See also electrospray ionization (ESI).

#### **atmospheric pressure ionization (API)** Ionization performed at atmospheric pressure by using atmospheric pressure chemical ionization (APCI), electrospray ionization (ESI), or nanoelectrospray ionization (nanoESI or NSI).

#### atmospheric pressure matrix-assisted laser

**desorption/ionization (AP-MALDI)** Matrix-assisted laser desorption/ionization in which the sample target is at atmospheric pressure.

See also matrix-assisted laser desorption/ionization (MALDI).

**Atmospheric Pressure Photoionization (APPI)** A soft ionization technique in which an ion is generated from a molecule when it interacts with a photon from a light source.

**atomic mass unit** Atomic Mass Unit (u) defined by taking the mass of one atom of carbon-12 as being 12u; unit of mass for expressing masses of atoms or molecules.

Automatic Gain Control<sup>™</sup> (AGC) Sets the ion injection time to maintain the optimum quantity of ions for each scan. With AGC on, the scan function consists of a prescan and an analytical scan.

See also ion injection time.

**autosampler** The device used to inject samples automatically into the inlet of a chromatograph.

**auxiliary gas** The outer-coaxial gas (nitrogen) that assists the sheath (inner-coaxial) gas in dispersing and/or evaporating sample solution as the sample solution exits the APCI, ESI, or H-ESI nozzle.

**auxiliary gas flow rate** The relative rate of flow of auxiliary gas (nitrogen) into the API source reported in arbitrary units.

**auxiliary gas inlet** An inlet in the API probe where auxiliary gas is introduced into the probe.

See also auxiliary gas and atmospheric pressure ionization (API).

**auxiliary gas plumbing** The gas plumbing that delivers outer coaxial nitrogen gas to the ESI or APCI nozzle.

**auxiliary gas valve** A valve that controls the flow of auxiliary gas into the API source.

#### В

**b** bit

**B** byte (8 b)

baud rate data transmission speed in events per second

BTU British thermal unit, a unit of energy

#### C

°C degrees Celsius

**CE** central electrode (of the Orbitrap analyzer);

European conformity. Mandatory European marking for certain product groups to indicate conformity with essential health and safety requirements set out in European Directives.

cfm cubic feet per minute

- **chemical ionization (CI)** The formation of new ionized species when gaseous molecules interact with ions. The process can involve transfer of an electron, proton, or other charged species between the reactants.
- **chemical ionization (CI) plasma** The collection of ions, electrons, and neutral species formed in the ion source during chemical ionization.

See also chemical ionization (CI).

**CI** See chemical ionization (CI).

CID See collision-induced dissociation (CID).

cm centimeter

cm<sup>3</sup> cubic centimeter

- **collision gas** A neutral gas used to undergo collisions with ions.
- **collision-induced dissociation (CID)** A method of fragmentation where molecular ions are accelerated to high-kinetic energy and then allowed to collide with neutral gas molecules such as helium or nitrogen. The collisions break the bonds and fragment the ions into smaller pieces.

- **consecutive reaction monitoring (CRM) scan type** A scan type with three or more stages of mass analysis and in which a particular multi-step reaction path is monitored.
- **contact closure connection** The cable connection is from the external peripheral device to the mass spectrometer contact closure pins (Start In and Ground). The external device sends the contact closure (start) signal to the mass spectrometer.
- **corona discharge** In the APCI source, an electrical discharge in the region around the corona discharge needle that ionizes gas molecules to form a chemical ionization (CI) plasma, which contains CI reagent ions.

See also chemical ionization (CI) plasma and atmospheric pressure chemical ionization (APCI).

- CPU central processing unit (of a computer)
- **CRM** See consecutive reaction monitoring (CRM) scan type.
- C-Trap curved linear trap
- <Ctrl> control key on the terminal keyboard

## D

**d** depth

Da dalton

DAC digital-to-analog converter

- **damping gas** Helium gas introduced into the ion trap mass analyzer that slows the motion of ions entering the mass analyzer so that the ions can be trapped by the RF voltage fields in the mass analyzer.
- **data-dependent scan** A scan mode that uses specified criteria to select one or more ions of interest on which to perform subsequent scans, such as MS/MS or ZoomScan.

DC direct current

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

**DS** data system

DSP digital signal processor

## Ε

ECD See electron capture dissociation (ECD).

EI electron ionization

electron capture dissociation (ECD) A method of fragmenting gas-phase ions for tandem mass spectrometric analysis. ECD involves the direct introduction of low energy electrons to trapped gas-phase ions.

See also electron transfer dissociation (ETD) and infrared multiphoton dissociation (IRMPD).

- electron multiplier A device used for current amplification through the secondary emission of electrons. Electron multipliers can have a discrete dynode or a continuous dynode.
- electron transfer dissociation (ETD) A method of fragmenting peptides and proteins. In electron transfer dissociation (ETD), singly charged reagent anions transfer an electron to multiply protonated peptides in the ion trap mass analyzer. This leads to a rich ladder of sequence ions derived from cleavage at the amide groups along the peptide backbone. Amino acid side chains and important modifications such as phosphorylation are left intact.

See also fluoranthene.

**electrospray ionization (ESI)** A type of atmospheric pressure ionization that is currently the softest ionization technique available to transform ions in solution into ions in the gas phase.

EMBL European Molecular Biology Laboratory

- <Enter> Enter key on the terminal keyboard
- **ESD** ElectroStatic Discharge. Discharge of stored static electricity that can damage electronic equipment and impair electrical circuitry, resulting in complete or intermittent failures.

ESI See electrospray ionization (ESI).

- **ESI flange** A flange that holds the <u>ESI probe</u> in position next to the entrance of the heated capillary, which is part of the API stack. The ESI flange also seals the atmospheric pressure region of the API source and, when it is in the engaged position against the spray shield, compresses the high-voltage safety-interlock switch.
- **ESI probe** A probe that produces charged aerosol droplets that contain sample ions. The ESI probe is typically operated at liquid flows of 1 µL/min to 1 mL/min without splitting. The ESI probe includes the ESI manifold, sample tube, nozzle, and needle.

**ESI source** Contains the ESI probe and the API stack.

See also electrospray ionization (ESI), ESI probe, and API stack.

**ESI spray current** The flow of charged particles in the ESI source. The voltage on the ESI spray needle supplies the potential required to ionize the particles.

**ESI spray voltage** The high voltage that is applied to the spray needle in the ESI source to produce the ESI spray current. In ESI, the voltage is applied to the spray liquid as it emerges from the nozzle.

See also ESI spray current.

ETD See electron transfer dissociation (ETD).

**eV** Electron Volt. The energy gained by an electron that accelerates through a potential difference of one volt.

**Extensible Markup Language** See XML (Extensible Markup Language).

**external lock mass** A lock that is analyzed in a separate MS experiment from your sample. If you need to run a large number of samples, or if accurate mass samples will be intermingled with standard samples, you might want to use external lock masses. These allow more rapid data acquisition by eliminating the need to scan lock masses during each scan.

See also internal lock mass.

#### F

**f** femto  $(10^{-15})$ 

- °F degrees Fahrenheit
- FAIMS (high-Field Asymmetric waveform Ion Mobility Spectroscopy) An optional device for separating ions at atmospheric pressure. FAIMS provides ion separation by taking advantage of compound-dependent changes in ion mobility at high electric field strengths.
- **FASTA database** A database format that represents either nucleic acid sequences or peptide sequences, and where base pairs or amino acids are represented using single-letter codes. A sequence in FASTA format begins with a single-line description, followed by lines of sequence data. FASTA databases all have the file extension .fasta.
- **Fast Fourier Transform (FFT)** An algorithm that performs a Fourier transformation on data. A Fourier transform is the set of mathematical formulas by which a time function is converted into a frequency-domain function and the converse.

FFT See Fast Fourier Transform (FFT).

- **firmware** Software routines stored in read-only memory. Startup routines and low-level input/output instructions are stored in firmware.
- **fluoranthene** A reagent anion that is used in an electron transfer dissociation (ETD) experiment.
- **forepump** The pump that evacuates the foreline. A rotary-vane pump is a type of forepump.
- Fourier transform (FT) The mathematical operation that converts the image current signal detected in an ICR trap or Orbitrap mass spectrometer to a set of m/z values. The Fourier components correspond to ion mass and the Fourier coefficients correspond to ion abundance.

Fourier Transform - Ion Cyclotron Resonance Mass Spectrometry (FT-ICR MS) A technique that determines the mass-to-charge ratio of an ion by measuring its cyclotron frequency in a strong magnetic field.

**fragment ion** A charged dissociation product of an ionic fragmentation. Such an ion can dissociate further to form other charged molecular or atomic species of successively lower formula weights.

- **fragmentation** The dissociation of a molecule or ion to form fragments, either ionic or neutral. When a molecule or ion interacts with a particle (electron, ion, or neutral species) the molecule or ion absorbs energy and can subsequently fall apart into a series of charged or neutral fragments. The mass spectrum of the fragment ions is unique for the molecule or ion.
- ft foot; feet
- FT Fourier Transformation

**FT-ICR MS** See Fourier Transform - Ion Cyclotron Resonance Mass Spectrometry (FT-ICR MS).

FTMS Fourier Transformation Mass Spectrometry

**full-scan type** Provides a full mass spectrum of each analyte or parent ion. With the full-scan type, the mass analyzer is scanned from the first mass to the last mass without interruption. Also known as single-stage full-scan type.

FWHM Full Width at Half Maximum

## G

**g** gram

**G** Gauss; giga  $(10^9)$ 

GC gas chromatograph; gas chromatography

GC/MS gas chromatography / mass spectrometer

GUI graphical user interface

## H

**h** hour

**b** height

**handshake** A signal that acknowledges that communication can take place.

**HCD** See Higher energy Collision-induced Dissociation (HCD).

**HCD cell** In a linear ion trap, Orbitrap, or hybrid MS, the collision cell where higher energy collision-induced dissociation (HCD) takes place.

See also:

Higher energy Collision-induced Dissociation (HCD)

**header information** Data stored in each data file that summarizes the information contained in the file.

#### heated electrospray See: H-ESI.

**H-ESI** Heated electrospray (H-ESI), a type of atmospheric pressure ionization, converts ions in solution into ions in the gas phase by using electrospray (ESI) in combination with heated auxiliary gas.

See also: auxiliary gas electrospray ionization (ESI)

#### Higher energy Collision-induced Dissociation

(HCD) Collision-induced dissociation that occurs in the HCD cell of the Orbitrap mass analyzer. The HCD cell consists of a straight multipole mounted inside a collision gas-filled tube. A voltage offset between C-Trap and HCD cell accelerates parent ions into the collision gas inside the HCD cell, which causes the ions to fragment into product ions. The product ions are then returned to the Orbitrap analyzer for mass analysis. HCD produces triple quadrupole-like product ion mass spectra.

#### High Performance Liquid Chromatography

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

**HPLC** See High Performance Liquid Chromatography (HPLC).

HV high voltage

Hz hertz (cycles per second)

## 

ID inside diameter

**IEC** International Electrotechnical Commission

IEEE Institute of Electrical and Electronics Engineers

**image current detection** The detection of ion motion by the charge (current) induced on one or more capacitive plates (outer electrodes).

in. inch

#### infrared multiphoton dissociation (IRMPD) In

infrared multiphoton dissociation (IRMPD), multiply charged ions consecutively absorb photons emitted by a infrared laser until the vibrational excitation is sufficient for their fragmentation. The fragments continue to pick up energy from the laser pulse and fall apart further to ions of lower mass.

See also electron capture dissociation (ECD).

**instrument method** A set of experiment parameters that define Xcalibur operating settings for the autosampler, liquid chromatograph (LC), mass spectrometer, divert valve, syringe pump, and so on. Instrument methods are saved as file type .meth.

**internal lock mass** A lock that is analyzed during the same MS experiment as your sample and is contained in the sample solution or infused into the LC flow during the experiment. Internal lock masses provide the most accurate corrections to the data.

See also external lock mass.

#### I/O input/output

- **ion gauge** Measures the pressure in the mass analyzer region (high-vacuum region) of the vacuum manifold.
- **ion injection time** The amount of time that ions are allowed to accumulate in the ion trap mass analyzer when AGC is off. With AGC on, the ion injection time is set automatically (up to the set maximum ion injection time) based on the AGC target value.

See also: Automatic Gain Control<sup>™</sup> (AGC).

- **ion optics** Focuses and transmits ions from the API source to the mass analyzer.
- **ion source** A device that converts samples to gas-phase ions.
- **ion-routing multipole (IRM)** The collision cell where higher energy collision-induced dissociation (HCD) takes place.
- **ion sweep cone** A removable cone-shaped metal cover that fits on top of the API ion transfer tube and acts as a physical barrier to protect the entrance of the tube.

**ion sweep gas** Extra nitrogen gas that flows along the axis of the API ion transfer tube (between the ion sweep cone and the capillary block) towards the API spray. The sweep gas flow is thus countercurrent to the flow of the ions.

See also ion sweep gas pressure.

**ion sweep gas pressure** The rate of flow of the sweep gas (nitrogen) into the API source. A measurement of the relative flow rate (in arbitrary units) to provide the required flow of nitrogen gas out from the Ion Sweep cone towards the API spray.

See also ion sweep gas.

**IRM** See ion-routing multipole (IRM).

**IRMPD** See infrared multiphoton dissociation (IRMPD).

**IS** interstage

#### Κ

**k** kilo (10<sup>3</sup>, 1000)

**K** kilo (2<sup>10</sup>, 1024)

#### KEGG Kyoto Encyclopedia of Genes and Genomes

kg kilogram

#### L

*l* length

L liter

LAN local area network

lb pound

LC See liquid chromatography (LC).

**LC/MS** See liquid chromatography / mass spectrometry (LC/MS).

LED light-emitting diode

LHe liquid helium

**liquid chromatography (LC)** A form of elution chromatography in which a sample partitions between a stationary phase of large surface area and a liquid mobile phase that percolates over the stationary phase.

#### liquid chromatography / mass spectrometry

(LC/MS) An analytical technique in which a high-performance liquid chromatograph (LC) and a mass spectrometer (MS) are combined.

LN2 liquid nitrogen

- **lock mass** A known reference mass in the sample that is used to correct the mass spectral data in an accurate mass experiment and used to perform a real-time secondary mass calibration that corrects the masses of other peaks in a scan. Lock masses with well-defined, symmetrical peaks work best. You can choose to use internal lock mass or external lock mass.
- **log file** A text file, with a .log file extension, that is used to store lists of information.

#### Μ

- $\mu$  micro (10<sup>-6</sup>)
- **m** meter; milli (10<sup>-3</sup>)
- **M** mega  $(10^6)$
- M<sup>+</sup> molecular ion
- **MALDI** See matrix-assisted laser desorption/ionization (MALDI).

#### matrix-assisted laser desorption/ionization

(MALDI) A method of ionizing proteins where a direct laser beam is used to facilitate vaporization and ionization while a matrix protects the biomolecule from being destroyed by the laser.

See also atmospheric pressure matrix-assisted laser desorption/ionization (AP-MALDI).

- MB Megabyte (1048576 bytes)
- $\mathbf{MH}^{+}$  protonated molecular ion
- **microscan** One mass analysis (ion injection and storage or scan-out of ions) followed by ion detection. Microscans are summed, to produce one scan, to improve the signal-to-noise ratio of the mass spectral data. The number of microscans per scan is an important factor in determining the overall scan time.

min minute

mL milliliter

**mm** millimeter

- **MRFA** A peptide with the amino acid sequence methionine–arginine–phenylalanine–alanine.
- MS mass spectrometer; mass spectrometry
- **MS scan modes** Scan modes in which only one stage of mass analysis is performed. The scan types used with the MS scan modes are full-scan type and selected ion monitoring (SIM) scan type.

#### MSDS Material Safety Data Sheet

- **MS/MS** Mass spectrometry/mass spectrometry, or tandem mass spectrometry is an analytical technique that involves two stages of mass analysis. In the first stage, ions formed in the ion source are analyzed by an initial analyzer. In the second stage, the mass-selected ions are fragmented and the resultant ionic fragments are mass analyzed.
- $MS^n$  scan mode The scan power equal to 1 to 10, where the scan power is the power *n* in the expression  $MS^n$ .  $MS^n$  is the most general expression for the scan mode, which can include the following:
  - The scan mode corresponding to the one stage of mass analysis in a single-stage full-scan experiment or a selected ion monitoring (SIM) experiment
  - The scan mode corresponding to the two stages of mass analysis in a two-stage full-scan experiment or a selected reaction monitoring (SRM) experiment
  - The scan mode corresponding to the three to ten stages of mass analysis (*n* = 3 to *n* = 10) in a multi-stage full-scan experiment or a consecutive reaction monitoring (CRM) experiment

See also MS scan modes and MS/MS.

- **multipole** A symmetrical, parallel array of (usually) four, six, or eight cylindrical rods that acts as an ion transmission device. An RF voltage and a DC offset voltage are applied to the rods to create an electrostatic field that efficiently transmits ions along the axis of the multipole rods.
- m/z Mass-to-charge ratio. An abbreviation used to denote the quantity formed by dividing the mass of an ion (in u) by the number of charges carried by the ion. For example, for the ion  $C_7H_7^{2+}$ , m/z=45.5.

#### Ν

**n** nano (10<sup>-9</sup>)

#### nanoelectrospray ionization (nanoESI or NSI) A

type of electrospray (ESI) that accommodates very low flow rates of sample and solvent on the order of 1 to 20 nL/min (for static nanospray) or 100 to 1000 nL/min (for dynamic nanoelectrospray, also called nanoESI nanoLC gradient separation).

#### See also:

atmospheric pressure chemical ionization (APCI) electrospray ionization (ESI)

- **NCBI** National Center for Biotechnology Information (USA)
- **NIST** National Institute of Standards and Technology (USA)

#### NMR Normal Mass Range

NSI See nanoelectrospray ionization (nanoESI or NSI).

#### 0

**octapole** An octagonal array of cylindrical rods that acts as an ion transmission device. An RF voltage and DC offset voltage applied to the rods create an electrostatic field that transmits the ions along the axis of the octapole rods.

#### **OD** outside diameter

**Orbitrap mass analyzer** The Orbitrap<sup>™</sup> mass analyzer consists of a spindle-shape central electrode surrounded by a pair of bell-shaped outer electrodes. Ions inside the mass analyzer orbit in stable trajectories around the central electrode with harmonic oscillations along it.



Two detection electrodes record an image current of the ions as they undergo harmonic oscillations. A Fourier transformation extracts different harmonic frequencies from the image current. An ion's mass-to-charge ratio m/z is related to the frequency f of its harmonic oscillations and to the instrumental constant k by:  $m/z = k/f^2$ 

#### OT Orbitrap

See Orbitrap mass analyzer.

OVC outer vacuum case

 $oldsymbol{\Omega}$  ohm

#### Ρ

**p** pico (10<sup>-12</sup>)

Pa pascal

- **parent ion** An electrically charged molecular species that can dissociate to form fragments. The fragments can be electrically charged or neutral species. A parent ion can be a molecular ion or an electrically charged fragment of a molecular ion. Also called a precursor ion.
- **parent mass** The mass-to-charge ratio of a parent ion. The location of the center of a target parent-ion peak in mass-to-charge ratio (m/z) units. Also known as precursor mass.

See also parent ion.

- PCB printed circuit board
- **PDA detector** The Photodiode Array detector is a linear array of discrete photodiodes on an integrated circuit chip. It is placed at the image plane of a spectrometer to allow a range of wavelengths to be detected simultaneously.

PE protective earth

**peak width** The distance across a peak measured at a selected peak-height level, in minutes or mass units. The peak-height level is usually specified as a percentage of the maximum peak height.

See also: peak width at half height

**peak width at half height** The full width of a peak at half its maximum height, sometimes abbreviated FWHM.

PID proportional / integral / differential

P/N part number

**p-p** peak-to-peak voltage

ppm parts per million

PQD pulsed-Q dissociation

**precursor ion** An electrically charged molecular species that can dissociate to form fragments. The fragments can be electrically charged or neutral species. A precursor ion (PR) can be a molecular ion or an electrically charged fragment of a molecular ion. Also known as parent ion.

**precursor mass** Mass of the corresponding precursor (or parent) ion or molecule.

psig pounds per square inch, gauge

PTM posttranslational modification

**pulsed Q dissociation (PQD)** Collision-induced dissociation that involves precursor ion activation at high Q, a time delay to allow the precursor to fragment, and then a rapid pulse to low Q where all fragment ions are trapped. The fragment ions can then be scanned out of the ion trap mass analyzer and detected. PQD eliminates the "1-3 Rule" low-mass cutoff for MS/MS data.

## 0

**quadrupole** A symmetrical, parallel array of four hyperbolic rods that acts as a mass analyzer or an ion transmission device. As a mass analyzer, one pair of opposing rods has an oscillating radio frequency (RF) voltage superimposed on a positive direct current (DC) voltage. The other pair has a negative DC voltage and an RF voltage that is 180 degrees out of phase with the first pair of rods. This creates an electrical field (the quadrupole field) that efficiently transmits ions of selected mass-to-charge ratios along the axis of the quadrupole rods.

#### R

RAM random access memory

**raw data** Uncorrected liquid chromatograph and mass spectrometer data obtained during an acquisition. Xcalibur and Xcalibur-based software store this data in a file that has a .raw file extension.

- **reagent carrier gas** Ultra-high-purity nitrogen gas used to transfer the reagent to the reagent ion source that is regulated by the backpressure regulator.
- **resolution** The ability to distinguish between two points on the wavelength or mass axis.
- **retention time (RT)** The time after injection at which a compound elutes. The total time that the compound is retained on the chromatograph column.

RF radio frequency

- **RF lens** A multipole rod assembly that is operated with only radio frequency (RF) voltage on the rods. In this type of device, virtually all ions have stable trajectories and pass through the assembly.
- **RF voltage** An AC voltage of constant frequency and variable amplitude that is applied to the ring electrode or endcaps of the mass analyzer or to the rods of a multipole. Because the frequency of this AC voltage is in the radio frequency (RF) range, it is referred to as RF voltage.

RMS root mean square

**RoHS** Restriction of Hazardous Substances. EU directive on the restriction of the use of certain hazardous substances in electrical and electronic equipment.

ROM read-only memory

- **rotary-vane pump** A mechanical vacuum pump that establishes the vacuum necessary for the proper operation of the turbomolecular pump. (Also called a roughing pump or forepump.)
- **RS-232** An accepted industry standard for serial communication connections. This Recommended Standard (RS) defines the specific lines and signal characteristics used by serial communications controllers to standardize the transmission of serial data between devices.
- **RT** An abbreviated form of the phrase retention time (RT). This shortened form is used to save space when the retention time (in minutes) is displayed in a header, for example, RT: 0.00-3.75.

#### S

s second

**sample loop** A loop of calibrated volume that is used to perform flow injection analysis.

- scan mode and scan type combinations A function that coordinates the three processes in the MS detector: ionization, mass analysis, and ion detection. You can combine the various scan modes and scan types to perform a wide variety of experiments.
- selected ion monitoring (SIM) scan type A scan type in which the mass spectrometer acquires and records ion current at only one or a few selected mass-to-charge ratios.

See also selected reaction monitoring (SRM) scan type.

selected reaction monitoring (SRM) scan type A scan type with two stages of mass analysis and in which a particular reaction or set of reactions, such as the fragmentation of an ion or the loss of a neutral moiety, is monitored. In SRM a limited number of product ions is monitored.

SEM secondary electron multiplier

**Serial Peripheral Interface (SPI)** hardware and firmware communications protocol

- **serial port** An input/output location (channel) for serial data transmission.
- **sheath gas** The inner coaxial gas (nitrogen), which is used in the API source to help nebulize the sample solution into a fine mist as the sample solution exits the ESI or APCI nozzle.
- **sheath gas flow rate** The rate of flow of sheath gas into the API source. A measurement of the relative flow rate (in arbitrary units) that needs to be provided at the sheath gas inlet to provide the required flow of sheath gas to the ESI or APCI nozzle.
- **sheath gas inlet** An inlet in the API probe where sheath gas is introduced into the probe.
- **sheath gas plumbing** The gas plumbing that delivers sheath gas to the ESI or APCI nozzle.

**sheath gas pressure** The rate of flow of sheath gas (nitrogen) into the API source. A measurement of the relative flow rate (in arbitrary units) that needs to be provided at the sheath gas inlet to provide the required flow of inner coaxial nitrogen gas to the ESI or APCI nozzle. A software-controlled proportional valve regulates the flow rate.

See also sheath gas.

- **sheath gas valve** A valve that controls the flow of sheath gas into the API source. The sheath gas valve is controlled by the data system.
- **signal-to-noise ratio (S/N)** The ratio of the signal height (S) to the noise height (N). The signal height is the baseline-corrected peak height. The noise height is the peak-to-peak height of the baseline noise.

SIM See selected ion monitoring (SIM) scan type.

- **skimmer** A vacuum baffle between the higher-pressure capillary-skimmer region and the lower-pressure region. The aperture of the skimmer is offset with respect to the bore of the ion transfer tube.
- **source CID** A technique for fragmenting ions in an atmospheric pressure ionization (API) source. Collisions occur between the ion and the background gas, which increase the internal energy of the ion and stimulate its dissociation.

**SPI** See Serial Peripheral Interface (SPI).

- **SRM** See selected reaction monitoring (SRM) scan type.
- **sweep gas** Nitrogen gas that flows out from behind the sweep cone in the API source. Sweep gas aids in solvent declustering and adduct reduction.

See also sweep gas flow rate.

**sweep gas flow rate** The rate of flow of sweep gas into the API source. A measurement of the relative flow rate (in arbitrary units) to provide the required flow of nitrogen gas to the sweep cone of the API source.

See also sweep gas.

**syringe pump** A device that delivers a solution from a syringe at a specified rate.

## T

T Tesla

**target compound** A compound that you want to identify or quantitate or that a specific protocol (for example, an EPA method) requires you look for. Target compounds are also called analytes, or target analytes.

TIC See total ion current (TIC).

TMP See turbomolecular pump.

**Torr** A unit of pressure, equal to 1 mm of mercury and 133.32 Pa.

**total ion current (TIC)** The sum of the ion current intensities across the scan range in a mass spectrum.

**tube lens offset** The voltage offset from ground that is applied to the tube lens to focus ions toward the opening of the skimmer.

See also source CID.

**Tune Method** A defined set of mass spectrometer tune parameters for the ion source and mass analyzer. Tune methods are defined by using the instrument software's tune window and saved as tune file.

A tune method stores tune parameters only. (Calibration parameters are stored separately, not with the tune method.)

**tune parameters** Instrument parameters whose values vary with the type of experiment.

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

TWA time weighted average

#### U

**u** atomic mass unit

UHV ultra high vacuum

#### ultra-high performance liquid chromatography

**(U-HPLC)** See High Performance Liquid Chromatography (HPLC).

#### Ultramark 1621 A mixture of

perfluoroalkoxycyclotriphosphazenes used for ion trap calibration and tuning. It provides ESI singly charged peaks at m/z 1022.0, 1122.0, 1222.0, 1322.0, 1422.0, 1522.0, 1622.0, 1722.0, 1822.0, and 1921.9.

UMR Universal Mass Range

## V

 $\mathbf{V}$  volt

VAC volts alternating current

**VDC** volts direct current

- **vacuum manifold** A thick-walled, aluminum chamber with machined flanges on the front and sides and various electrical feedthroughs and gas inlets that encloses the API stack, ion optics, mass analyzer, and ion detection system.
- **vacuum system** Components associated with lowering the pressure in the mass spectrometer. A vacuum system includes the vacuum manifold, pumps, pressure gauges, and associated electronics.
- **vent valve** A valve that allows the vacuum manifold to be vented to air or other gases. A solenoid-operated valve.

#### W

 $\mathbf{w}$  width

W watt

**WEEE** European Union Waste Electrical and Electronic Equipment Directive. Provides guidelines for disposal of electronic waste.

## X

#### XML (Extensible Markup Language) A

general-purpose markup language that is used to facilitate the sharing of data across different information systems, particularly via the Internet.

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