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## **QUADERA®** Help

#### Program version 4.61, February 2015

Welcome to QUADERA®, the software for controlling the mass spectrometers QMG220 and QMG700. QUADERA® is a Windows application based on Microsoft's .NET framework and other contemporary technologies. The user interface is state of the art and provides access to settings and data.



- Copyrights: Copyrights and trademarks,
- <u>License agreement</u>: License agreement for the QUADERA® software,
- Resources to access the online Help: The online Help contains all the information required for operating QUADERA®.

Please read the "Setting Up" section to easily configure QUADERA® and the devices.

#### NOTE:

Read the QUADERA® Release Notes. They list new features, bugfixes, known problems and limitations of QUADERA®. In addition, the Release Notes give important information on installing and configuring QUADERA®, on the operating system, and on the network settings.

#### Opening the Release Notes:

After installing QUADERA® with the default settings, proceed as follows to open the Release Notes:

- Via the Windows start menu: Program Files > QUADERA > Readme
- Open the file "Readme.html" in the <u>directory for programs and settings</u>.

# **License Agreement**

Please be sure to read the conditions of this Software License Agreement.

Please direct any inquiries in writing to the following address:

#### USA:

INFICON Inc. Two Technology Place E. Syracuse NY 13057 USA

#### **Europe and Asia:**

INFICON Aktiengesellschaft Abteilung KA LI-9496 Balzers Liechtenstein

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- 1. LICENSEE has purchased an equipment and/or a component from INFICON hereafter referred to as HARDWARE.
- 2. The SOFTWARE allows the HARDWARE to be computer controlled.
- 3. This contract defines the conditions under which INFICON grants the LICENSEE the right to use the SOFTWARE required for computer control of the HARDWARE.

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#### **TRADEMARKS**

QUADERA® is a registered trademark of INFICON.

Microsoft® Visual Studio® Tools for Applications (VSTA) is a registered trademark of Microsoft Corp.

### **Cross-References from Manuals**

In this topic you find cross-references from manuals that refer to the QUADERA® Online-Help. Click on the corresponding link below to display the required topic:

#### Cross-references from the "PrismaPlus" manual

- Cross-reference #001: <u>System configuration</u>
- Cross-reference #002: Commissioning
- Cross-reference #003: Measuring mode
- Cross-reference #004: EXTERNAL PROTECTION
- Cross-reference #005: <u>Using the analog and digital interfaces</u>
- Cross-reference #006: Optimizing the ion source sensitivity
- Cross-reference #007: <u>Tuning the RF generator</u>

# Migrating from Quadstar to QUADERA

### Migrating from Quadstar to QUADERA®

Quadstar is an application software for the QMS 422/421 and QMS 200 Prisma™ quadrupole mass spectrometers. QUADERA® and Quadstar share some basic capabilities. However, they sometimes differ in the used terminology, and especially in the functionality and the tools. Once you know these differences you will be able to migrate to QUADERA® easily.

Overview of the differences in the used terminology

Overview of the differences in the available tools and functions

### Overview and Differences in the Used Terminology

The terms and concepts of Quadstar and QUADERA® differ in some ways. Many terms have a similar meaning, but they are named differently. The table below contains the terms used in Quadstar and the equivalent terms used in QUADERA® .

Quadstar term	QUADERA® term
Channel	Measurement task
Channel parameter editor	Recipe editor
Mass spectrometer	<u>Device</u>
Measurement	Measurement project
Measurement parameter file	Measurement project template

#### Overview and Differences in the Available Functions

Quadstar comprises a package of several main programs (measurement program, display program, analysis program, etc.). These programs are called up and closed individually as the need arises. In QUADERA®, on the other hand, the entire functionality is always available. It is no longer necessary to call up or close individual components. QUADERA® allows you to display several measurement projects at a time and also to display different views of one measurement project.

Notation: xxx > yyy > zzz means "In the main menu, select the item xxx. In the following submenu, select the item yyy. Then select the item zzz".

Function	Quadstar	QUADERA®
Select the simulation mode	"Parset" program: Setup > General > Simulation Mode > Intern	<u>Device &gt;</u> <u>Communication</u> <u>Settings &gt; Simulator</u>
System information	For each main program: File > About	Help > About
Establish a connection to the device	For each main program: Comm > Connect	<u>Device &gt; Connect</u>
Open a measurement project template for Scan	Via the file manager in the "Measure" program: Scan > Analog	Via the <u>Start page</u>
Open a measurement project template for MID	Via the file manager in the "Measure" program: MID > Versus Time	Via the <u>Start page</u>
Start/stop a Scan measurement	Via the file manager in the "Measure" program: Scan > Analog > Operation > Go/Halt	<u>Device &gt; Run</u>
Start/stop a MID measurement	Via the file manager in the "Measure" program: MID > Versus Time > Operation > Go/Halt	<u>Device &gt; Run</u>
Save measuring data	Manually in the file manager: File > Save Cycle Data	Automatically
Open an existing measurement project	"Dispsav" program: Scan > Analog Data	File > Open

(Scan measurement)		
Open an existing measurement project (MID measurement)	"Dispsav" program: Process > Cycles	File > Open
Edit measurement parameters	Via the file manager and the channel parameter editor in the "Parset" program	Directly in the corresponding working area of the opened measurement project (Recipe Editor)
Automate measurements and analyses	Via the sequencer (command interpreter with a specific syntax) in the "Parset" program	In parts implemented via the <u>VBA editor</u> and the use of <u>macros</u>
User access	Via the "Accessc" administration program directly in Quadstar	Handled by the operating system of the PC on which QUADERA® has been installed

### **QUADERA**

#### Introduction

### **Product Description**

### **Product Description**

QUADERA® is a powerful operation and analysis software for the following quadrupole mass spectrometers:

- QMG220
- QMG700

QUADERA® allows you to perform a qualitative and quantitative analysis.

QUADERA® simplifies the operation of the mass spectrometer, improves the reproducibility of the results, and allows you to store all relevant parameters and data. In addition, it also checks the consistency of specific parameters and issues a warning in the case of an error.

QUADERA® allows you to save and to document measuring data, to reload these data and to display the reloaded data in various ways (table, bar graph, trend etc.).

### **Main Features**

- Easy operation via graphical user interface
- Powerful measuring programs for qualitative and quantitative analysis
- Analysis of measuring data while a measurement is running
- Display of multiple measurement tasks in a table, as a bar graph, or as a trend
- Measurements can be documented
- Service functions
- Online parametrization of the mass spectrometer
- Automatic electrometer range switching

### Scope of Delivery

#### Software

- License agreement and license key.
- CD-ROM with QUADERA®. The supplied installation program will create the required folders and copy various files into these folders.
- Measurement project templates are supplied for all types of measurement.

Directories created during installation under Windows XP with the default settings

- Programs and settings: "C:\Program Files\QUADERA"
- Example files: "C:\Documents and Settings\[User]\My Documents\My OUADERA\Data"
- Measurement project templates: "C:\Program Files\QUADERA\[QMG]"
- Tool programs: "C:\Program Files\QUADERA\Tools"
- Simulator: "C:\Program Files\[QMG]Sim"
- Files created by the user: "C:\Documents and Settings\[User]\My Documents\My QUADERA\Data"
- Computer specific settings: "C:\Documents and Settings\All Users\Application Data\INFICON\QUADERA\[Version]"
- User specific settings: "C:\Documents and Settings\[User]\Application Data\INFICON\QUADERA\[Version]"
- Scripting: "C:\Documents and Settings\[User]\My Documents\My QUADERA\Scripting"

#### Notes:

[User] represents your registered profile, [Version] indicates the currently installed version of QUADERA®, [QMG] specifies the mass spectrometer, i.e. QMG220, QMG700.

Directories created during installation under Windows 7 with the default settings

- Programs and settings: "C:\Program Files\QUADERA"
- Example files: "C:\Users\[User]\Documents\My QUADERA\Data"
- Measurement project templates: "C:\Program Files\QUADERA\[QMG]"
- Tool programs: "C:\Program Files\QUADERA\Tools"
- Simulator: "C:\Program Files\QUADERA\[QMG]Sim"
- Files created by the user: "C:\Users\[User]\Documents\My QUADERA\Data"
- Computer specific settings: "C:\Users\All Users\QUADERA\[Version]"
- User specific settings:
- "C:\Users\[User]\AppData\Roaming\QUADERA\[Version]"
- Scripting: "C:\Users\[User]\Documents\My QUADERA\Scripting"

Notes:

[User] represents your registered profile, [Version] indicates the currently installed version of QUADERA®, [QMG] specifies the mass spectrometer, i.e. QMG220, QMG700.

#### **Cables and Accessories**

- Ethernet cable with crossed wires for direct connection of the mass spectrometer to a PC
- Normal Ethernet cable for direct connection of the mass spectrometer to a network

### **System Requirements**

In order to install the QUADERA® software on a PC, the following minimum requirements for hardware and software must be met:

#### Hardware for operating system Windows XP

- Processor: Intel P3 1.5 Ghz (or other equivalent processors), recommended P4 3 GHz
- Main memory: 512 MB, recommended 1 GB
- Free space on the harddisk: 100 MB to install the program, additional space for the measurement data
- Graphics card: Resolution 1024 x 768 pixels or higher, at least 256 colors
- CD-ROM drive
- Color monitor
- Interface for the mass spectrometer (Ethernet 10/100)

#### Hardware for operating system Windows 7

• Adhere to the QUADERA® Release Notes.

#### **Software**

- Operating system Windows XP Professional with Service Pack 2 or 3
- Operating system Windows 7
- Note: No other Windows operating systems are supported.

### **Getting Help**

#### Calling Help

If you need help during your work, you may utilize the following resources:

- Select the Help menu and click Contents or Index, or Press the function key [F1].
- 2. If the **Contents**, **Index** and **Search** tabs are not displayed in the Help window, click Show
- 3. Perform one of the following steps in the Help window:
  - Click the **Contents** tab to display the table of contents for the help file.
  - Click the **Find** tab to search for specific key words. Enter the required words and then click Search.
  - Click the **Index** tab to search for specific words or to choose from a key word list.

You can control the number of the found topics by adding key words to the search string or by removing them from the string. This way you can restrict the search result in the list to the relevant topics and key words.

In addition, you can use the Windows start menu to open the online help:

- 1. Click on the Windows **START** button and select **Programs**.
- 2. Select the program group QUADERA and click on QUADERA Help.

### **Changing the Display of a Help Topic**

The Help window uses the same settings for fonts, font colors and background colors as the browser installed on your computer. These settings and other options depend on the type and version of the installed browser. You can change the appearance of the help topics in the Help window by changing the settings for fonts and colors.

- 1. Open the Help window.
- 2. In the **Help** window, click **Options** and then **Internet Options**
- 3. In the **General** tab, click **Accessibility** and then select **Ignore colors specified** on Web pages.
- 4. Click **OK**.
- 5. Perform one of the following actions in the Internet Options dialog box:
  - Changing the background or text color in the help:
     In the General tab, click Colors... and then select the required options.
  - Changing the font in the help: In the **General** tab, click **Fonts...** and then select the required options.

#### NOTE:

Any change in the font and background color of the help topics in the Help window will also affect the font and background color of websites displayed by Microsoft Internet Explorer.

Further information on the settings and options available in your browser can be found in the help file for your browser.

### **Printing a Help Topic**

### Printing the current topic

- 1. In the Help window, click **Print**
- 2. Select the required printing options.

### **Printing several topics**

- In the Help window, click the Contents tab.
   If the Contents tab is not displayed, click Show
- 2. Select the required heading and then click Print
- 3. Perform one of the following actions:
  - In order to print the current page, select **Print selected topic**.
  - In order to print all topics under the selected heading, select **Print the** selected heading and all subtopics.
  - 4. Select the required printing options.

### **Further Information**

You can check which version of QUADERA® is installed on your computer and determine the product ID and the license key of your program. In addition, you can call up system information.

• In the **Help** menu, select **About**...

### Installing and Uninstalling QUADERA

### **Installation Program SETUP**

QUADERA® comes as a compressed file on a CD-ROM. SETUP copies and unpacks the QUADERA® program files and creates the required directories on the selected drive (pay attention to the system requirements).

The installation directory (default: C:\Program Files\QUADERA) contains all QUADERA® program files. Special subdirectories are created for all other files.

#### NOTE:

If required you can change the locations of the special subdirectories after the installation has been completed (<u>menu Tools>Options</u>).

SETUP is used for the following tasks:

- Installing QUADERA®,
- Updating QUADERA®,
- <u>Upgrading</u> QUADERA®.

#### NOTES:

Uninstalling QUADERA prior to installing a new version will most often result in the best installation.

Unrestricted use of QUADERA® requires a valid license key.

### Installing

#### NOTE:

Unrestricted use of QUADERA® requires a valid license key.

#### NOTE:

In order to install QUADERA®, a user account with administrator access rights is required.

Proceed as follows to install QUADERA®:

- 1. Check to make sure that the system requirements are met.
- 2. Start Windows and close all other applications. Pay attention to the instruction manual for your operating system.
- 3. Insert the OUADERA® installation CD into the CD-ROM drive.
  - The installation procedure should start automatically after a few seconds.
  - If the installation procedure does not start within 30 seconds, the autostart function of the drive may be disabled. In this case, use Windows Explorer to access the CD-ROM drive and execute the **index.html** file.
- 4. Follow the instructions of the installation program and enter all required parameters or accept the respective default settings.

#### NOTE:

After installing QUADERA®, you have to set up the following:

- The communication between the PC and the mass spectrometer,
- The configuration of the mass spectrometer.

An account with administrator access rights is **not** required in order to operate QUADERA®.

### **Setting Up**

NOTE: By default, QUADERA® works with a <u>simulator</u> that is installed together with the software. After the installation procedure, QUADERA® is basically ready for operation and it can be used without a device.

NOTE: Adhere to the QUADERA® Release Notes.

Proceed as follows to set up QUADERA®:

- 1. Start QUADERA®.
- 2. In the **Device** menu, click **Device Setup...**. The "Device Setup" dialog opens. Click **Search**.
- 3. The search scans the network for running QMG mass spectrometers. Click **Search** again, if all mass spectrometers are not found, to start another search.
- 4. In the "Device Search" dialog select a device (or devices) and click **Add**. Close the dialog.
- 5. Click **Apply** in the 'Device Setup' dialog to acknowledge the input. QUADERA will now connect to each device, acquire the Device Name, and disconnect from each device.
  - Any device unable to connect will be named 'unknown'. On any future 'Connect', the Device Name will be acquired and assigned.
  - 6. Click the **Configure** button to change the name of any device.
- 7. **Apply** any changes and close the dialog.
- 8. QUADERA® is now configured for the connection with the mass spectrometer(s).
- 9. If necessary adjust the configuration:
  - Use the <u>basic device settings</u> in the device status view ("<u>Device Configuration View</u>" icon) to adjust the configuration. Normally these settings have already been performed in the factory.

QUADERA® now allows more than one device to be connected and acquiring data simultaneously if properly licensed ('Multiplexing' license). This multiple device design, known as Multisensor, can run for an extended period of time but it is recommended to limit duration and/or quantity of data collected in any one session.

NOTE: Multisensor can be enabled through the Options menu and must be enabled to use the Multiplexing add-in.

# **Adjusting the Device Settings**

#### NOTE:

Normally most device settings have already been performed in the factory. The Device Name is one setting that can be customized.

Proceed as follows to adjust the device settings:

- 1. Connect QUADERA® with the device.
- 2. In the device status view, click on the "Device Configuration View" icon. The "Device Configuration" window opens.
- 3. Adjust the parameters to the device settings. The following table list the available parameters.
- 4. Click [Close] to close the "Device Configuration" window.

### NOTE:

Select only components that are actually installed in your device.

Parameter		Range	Description
•	Device Name	Edit box	The Device Name used to label the device.
•	Device MAC	Automatically detected	The unique hardware address of the device.
•	Auto Connect at Startup	Dropdown list	Selection of feature to automatically connect device at QUADERA® startup.
•	Analyser Detector Type	Dropdown list	Selection of the detector type (installed gauge head):  • Faraday: only "Faraday" is available in recipes,
			<ul> <li>SEM: "Faraday" and "SEM" are available in recipes.</li> </ul>
•	Ion Source Type	Dropdown list	Selection of the ion source type:
			<ul> <li>Axial: Axial ion source (only QMG700),</li> </ul>
			Crossbeam: Cross-Beam ion

			<ul> <li>source,</li> <li>Grid: Grid ion source,</li> <li>SPM: Sputter Process Monitor,</li> <li>High sensitivity (only QMG220),</li> <li>SpecPos (only QMG700),</li> <li>SpecNeg (only QMG700).</li> </ul>
•	Protection	Dropdown list	Monitoring of filament and SEM.
			If a pressure gauge is installed:
			<ul> <li>InternalOff: use QUADERA® to switch filament and SEM manually on and off,</li> </ul>
			<ul> <li>ExternalOnOff: an external system, such as a pressure gauge, protects filament and SEM. They are automatically switched on and off as determined by the parameters "Total Pressure Level On/Off".</li> </ul>
			ExternalOff: an external system, such as a pressure gauge, protects filament and SEM. They are automatically switched off as determined by the parameter "Total Pressure Level Off". Use QUADERA® to switch filament and SEM manually on.
			If no pressure gauge is installed: the protection input of the device is used.
•	QMA	For QMG220: Automatically detected	Indicates the installed QMA.
		For QMG700: Dropdown list	Selection of the QMA.
•	QMH	For QMG220: Automatically detected	Indicates the installed RF device, which defines the mass range.
		For QMG700: Dropdown list	Selection of the QMH, depends on the installed QMA.
•	Mass Range	Automatically detected	Indicates the mass range in [amu], depends on the installed QMA and QMH.
•	Simulation Mode	Dropdown list	Defines the simulation mode of the device:
			• Off,

- Internal,
- External.

#### NOTE:

The <u>software simulation</u> (local simulation on the PC) requires no real device.

• 10220, or 10700

Automatically detected

Indicates whether an Input/Output-module (IO220 or IO700) has been detected or not.

 Total Pressure Level Off Number > 0

Only valid when a total pressure gauge is installed.

Monitoring the QMG via total pressure measurement: pressure threshold when filament and SEM switch automatically off (pressure rise).

The parameters "Total Pressure Level Off" and "Total Pressure Level On" should form a hysteresis to avoid repeated switching when minor pressure fluctuations occur.

Total Pressure Level On Number > 0

Only valid when a total pressure gauge

is installed.

Monitoring the QMG via total pressure measurement: pressure threshold when filament and SEM switch automatically on (decrease of pressure).

Total Pressure RS 485 Address Valid address

Only valid when a total pressure gauge is installed.

Total pressure measurement: address of the installed digital pressure gauge.

Note that the pressure gauge is only recognized when the device is turned on (no "hot-plug").

• Total Automatically Pressure Type detected

Only valid when a total pressure gauge is installed.

Total pressure measurement: type of the installed analog/digital pressure gauge.

Note that the pressure gauge is only recognized when the device is turned on (no "hot-plug").

NOTE: Buttons are available to degas the Filament Ion Source and Total Pressure Gauge filament (if present). Degas of the Filament Ion Source can be started and stopped manually or run for a duration of time. The Degas function can also be accessed from the All Device Status View.

#### **Version Number**

The product version of QUADERA® is indicated by a two-digit number shown as x.yz, e.g. 1.12.

- "1" indicates the major version,
- "12" indicates the minor version.

In the **Help>About**... menu you find the <u>version number of your software</u> and further information, as well as product extensions.

#### **Update**

A software update is a maintenance release of the software within the same major version. The minor version has been increased (e.g. from 1.12 to 1.13). Updates contain new features and additional functions or they fix software bugs that have been discovered.

### Upgrade

A software upgrade represents an extensive revision of the software and is marked as a new major version (e.g. from version 1 to 2). Upgrades contain extensive revisions and they offer an extended and improved range of functions for the software.

# **Updating**

The version number allows you to find out if an <u>update or upgrade</u> for QUADERA® is available.

Proceed as follows to update/upgrade your QUADERA® version:

- 1. Start Windows and close all other applications.
- 2. Insert the CD with the latest product release into the CD-ROM drive.
- 3. Follow the instructions of the installation program and enter all required parameters or accept the respective default settings.

### Uninstalling

#### NOTE:

In order to uninstall QUADERA®, a user account with administrator access rights is required.

Proceed as follows to uninstall QUADERA®:

- 1. Exit QUADERA®.
- In the Windows Start menu, select Control Panel > Add or Remove
   Programs.

   In Windows 7: Start menu Control Panel > Programs > Uninstall a program
- 3. Select QUADERA®.
- 4. Click [Remove] or Uninstall (Win 7). You are asked to confirm the action.
- 5. Click **[OK]** or **[Continue]** (Win 7) to uninstall the QUADERA® application.

#### NOTE:

Files which have been created automatically by the software and user files remain on the harddisk. If you want to remove these files you may do so manually. In this case, adhere to the <a href="QUADERA® Release Notes">QUADERA® Release Notes</a>.

# **Operating Concept**

# **Basics for Operation**

For a basic understanding of the operating routines and procedures in QUADERA® it is necessary to know the object structures that are visible to the user.

Object	Description
QUADERA®	Instance of the QUADERA® software
Toolboxes	The toolboxes provide tools which allow you to adjust the working area according to the measurement task.
Software device	Image of the real <u>device</u> in QUADERA®
Device	Mass spectrometer
Measurement project	Contains all instruments required to perform a specific application.
	One device is assigned to each measurement task. It is possible that several measurement projects relate to the same device.
Recipe	Sequence or collection of measurement tasks
Measurement task	Configurable measurement task. It is the basic component of a recipe and contains the measuring mode and all parameters required for its definition (e.g. MID, MCD, Scan).
Working area	Part of the graphical user interface of QUADERA®. The working area is used for the following:
	<ul> <li>To display the recipe editor. This working area is present in the most <u>recipes</u> and cannot be removed by the user.</li> </ul>
	<ul> <li>As a container for the <u>sections</u> and the related measuring data displays. The user can add several working areas to a recipe.</li> </ul>
Section	Part of the <u>working area</u>
	Each working area - except for the working area used to display the recipe definition - can be divided into so-called sections by the user. Each section can be filled with a graphical object (e.g. measuring data display).
Chart element	Graphical object which connects the data of a measurement task with a data display. A chart appears in the section.

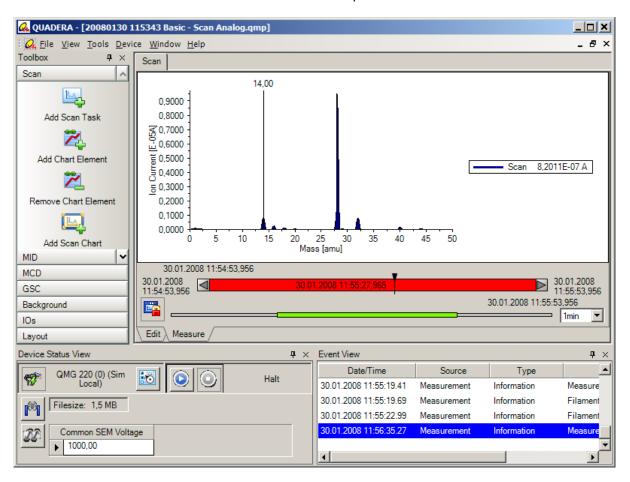
The data display in QUADERA® is strongly related to the corresponding measurement tasks. The appropriate <u>tool</u> allows you, for instance, to create or remove a measurement task directly in the data display of the section.

Example for the relation between measurement task and data display In order to observe the change of several gases with time, the MID (Multiple Ion Detection) type of measurement is especially suitable. In this example, one measurement task relates to a mass whose intensity is to be measured, and it defines the parameters required for the measurement. The recipe unites all measurement tasks, i.e. the masses to be observed. During a measurement, the measurement tasks are performed one after the other, the readings are collected and stored in the related measurement project. The repeated execution of a measurement task results in a sequence of data which show the course of the related mass signals as a function of the time. The measuring data which are obtained in a measurement task can be displayed graphically in a chart in the section (e.g. as a curve or a bar chart). As a result, they represent a chart element.

### **Operating Elements**

#### **User Interface**

The QUADERA® window is divided into several areas. For each area, a tooltip displays brief information. For this, move the mouse pointer to the required area in the figure below. For more detailed information, click the respective area.



Example of the QUADERA® user interface

# **Screen Elements**

Name	Example	Description
Checkbox		You can select Yes (with checkmark) or No (without checkmark) as follows:
		<ul> <li>Press the space bar,</li> </ul>
		Click the checkbox with the mouse.
Radio buttons	<b>9</b> 0	Radio buttons allow you to select one option at a time. You can select the required option as follows:
		<ul> <li>Press the space bar,</li> </ul>
		<ul> <li>Click the required button with the mouse.</li> </ul>
		This will automatically reset the previously selected button.
Dropdown	deutsch 🔻	Select the required list item as follows:
list	english deutsch	<ul> <li>Click the currently displayed item to open the entire dropdown list,</li> </ul>
		<ul> <li>Click the required item with the mouse. The dropdown list closes and only the selected item is displayed.</li> </ul>
Spin buttons	2	Increase or decrease the displayed value as follows:
		<ul> <li>Click one of the spin buttons to increase (arrow up) or decrease (arrow down) the value by one,</li> </ul>
		<ul> <li>Click the input field next to the spin buttons and enter the required value directly.</li> </ul>
Tooltips	Device configuration view.	The tooltip is a small box in the graphical user interface and displays supplementary information on an item, such as symbols. A tooltip appears when the user hovers the mouse pointer over an item, without clicking it.

# **Mouse Actions**

Action	Description (default assignment for the mouse buttons)
Click	Position the mouse pointer on the required object (file, text, figure etc.). Then press the left mouse button.
Double- click	Position the mouse pointer on the required object. Then press the left mouse button twice in rapid succession.
Drag & drop	Position the mouse pointer on the required object. Press the left mouse button and keep it pressed. Drag the object to the new position (destination) and then release the mouse button. The object will be put down at the destination.
Right mouse button	Position the mouse pointer on the required object. Then press the right mouse button. In general, this will open a context menu offering some object related functions to you.

# **Keyboard Shortcuts**

### NOTE:

The following table describes the default settings for the keyboard shortcuts. You can <u>customize the keyboard shortcuts</u> to suit your needs.

Key	Action
F1	Call up help
CTRL+O	Open a measurement project
ALT+F4	Exit the application
ALT+F8	Call up the Macros dialog

### **Customizing the Keyboard Shortcuts**

By default, QUADERA® already contains predefined keyboard shortcuts. You may change or extend these settings to suit your needs. As an example, you may do one of the following:

- Assign keyboard shortcuts to frequently used commands and macros,
- <u>Delete keyboards shortcuts</u> which are no longer needed.

#### Assigning keyboard shortcuts

Proceed as follows to assign a keyboard shortcut:

- 1. Call up the context menu for the menu bar.
- 2. Click Customize...
- 3. Click **Keyboard...**
- 4. Select a command category from the list.
- 5. Click a command in the command list. The **Specify a Shortcut** field displays the keyboard shortcut that is currently assigned to the selected command.
- 6. Select a keyboard shortcut in the **Specify a Shortcut** field.
- 7. Click **Assign**. The keyboard shortcut is assigned to the selected command.

If the selected keyboard shortcut has already been assigned to another command, the latest assignment will replace the previous one.

Click **Reset All...** to reset all keyboard shortcuts to the default assignments.

#### **Deleting keyboard shortcuts**

Proceed as follows to delete a keyboard assignment:

- 1. Call up the Context menu for the menu bar.
- 2. Click Customize...
- 3. Click Keyboard...
- 4. Select a command category from the list.
- 5. Click a command in the command list. The **Specify a Shortcut** field displays the keyboard shortcut that is currently assigned to the selected command.

6. Click **Remove**. The assignment between the keyboard shortcut and the command is removed.

Click **Reset All...** to reset all keyboard shortcuts to the default assignments.

# **User Interface**

# **Title Bar**

The title bar is a subarea of the QUADERA® user interface.

The title bar displays the following items:

- Program symbol: Click this symbol to call up the <u>title bar menu</u>.
- Program name
- Currently loaded file (measurement project)

### Menu Bar

The menu bar is a subarea of the QUADERA® user interface.

Each menu contains a list of commands. The menu bar allows you to call up all functions of QUADERA®. The following main menus are available:

<u>File</u>	File and printer related functions	
<u>View</u>	View settings	
<u>Tools</u>	Additional functions	
<u>Device</u>	Device related functions	
Window	Management and arrangement of the windows	
<u>Help</u>	Help functions	

QUADERA® main menus

#### File menu

The **File** menu contains the following functions:

- Open
- Export
  - <u>ASCII</u>
- Save as Template...
- <u>Close</u>
- Recent Files
- Exit

#### View menu

The **View** menu contains the following functions:

- Show Start Page
- Event View
- Device Status
- All Device Status
- <u>Toolbox</u>

#### Tools menu

The **Tools** menu contains the following functions:

- Programming
  - Macros...
  - Create Add-in...
  - Add-in Manager...
- Options...
- Spectra Library

#### Device menu

The **Device** menu contains the following functions:

- Connect
- Run
- Device Setup...

#### Window menu

The **Window** menu contains the following functions:

- Arrange Icons
- <u>Cascade</u>
- Close All Windows
- <u>Tile Horizontally</u>
- Tile Vertically
- Minimize All Windows
- Window List

#### Help menu

The **Help** menu contains the following functions:

- Contents
- Index
- Report an Error...
- About...

# **Options**

Use the "Options..." window to perform the following settings:

- Specifying the path (file location) for various file types used by Quadera® ("File Locations" tab)
- Changing the line thickness of curves in charts ("Display" tab)
- Enabling Multisensor, the ability to connect to and collect from more than one device. As of QUADERA version 4.20 this must be enabled (and licensed) to use either Multisensor or Multiplexing (from VSTA).

### **Toolbox**

#### **Toolbox**

The toolbox is a subarea of the QUADERA® user interface.

The toolbox is used to customize the working area of a measurement project. The main task is to create new objects. The toolbox is subdivided into different groups according to the subject. One tool can be used in several groups. Click the respective button to open the required toolbox.

### NOTE:

Toolboxes may contain varying tools depending on the configuration of QUADERA®.

Refer to the <u>alphabetical list of tools</u> if you search for a specific tool.

### **Applying Tools**

### Applying via drag & drop

- 1. Open the required toolbox.
- 2. Use the buttons and if necessary. The toolbox is scrolled up and down, respectively, to display the desired tool.
- 3. Drag the required tool into the section:
  - A mouse pointer shaped as indicates that the selected tool is applicable,
  - A mouse pointer shaped as **O** indicates that the selected tool is not applicable.

**Alphabetical list of tools** 

# **List of Tools**

Alphabetical list of all tools which are available in QUADERA  ${\mathbin{\bf @}}$  :

Icon	Name	Description
*	Add 'Analog Input' Editor	Add an analog input editor to the section.
	Add Analog Input Task	Depends on the working area into which you drag the tool:
		<ul> <li>Dragging the tool to the recipe editor:         Add a measurement task to the recipe.         The task uses an analog input channel, such as the quadrupole controller QC ("EXT IN").     </li> </ul>
		<ul> <li>Dragging the tool to the chart:         Add a measurement task to the recipe using an analog input channel. Display the data of this measurement task in the chart.     </li> </ul>
		Refer to the operating instructions of your QMG mass spectrometer.
*	Add 'Analog Output' Editor	Add an analog output editor to the section.
	Add Chart Element	Connect an existing measurement task with a chart.
*	Add 'Digital Input' Editor	Add an digital input editor to the section.
*	Add 'Digital Output' Editor	Add an digital output editor to the section.
[186]	Add MCD Chart	Add an (empty) MCD chart to the section.
		Only available for MID recipes.
	Add MCD Task	Depends on the working area into which you drag the tool:
		<ul> <li>Dragging the tool to the recipe editor: Add a MCD measurement task to the recipe.</li> </ul>
		<ul> <li>Dragging the tool to the chart:         Add a MCD measurement task to the recipe. Display the data of this measurement task in the chart.     </li> </ul>
		Only available for MCD recipes.

	Add MID Chart	Add an (empty) MID chart to the section.
		Only available for MID recipes.
E-G	Add MID Task	Depends on the working area into which you drag the tool:
		<ul> <li>Dragging the tool to the recipe editor:         Add a MID measurement task to the         recipe.</li> </ul>
		<ul> <li>Dragging the tool to the chart:         Add a MID measurement task to the recipe. Display the data of this measurement task in the chart.     </li> </ul>
		Only available for MID recipes.
1111	Add Peak Task	Depends on the working area into which you drag the tool:
		<ul> <li>Dragging the tool to the recipe editor:         Add a peak measurement task to the         recipe.</li> </ul>
		<ul> <li>Dragging the tool to the chart:         Add a peak measurement task to the recipe. Display the data of this measurement task in the chart.     </li> </ul>
		Only available for scan recipes (see <u>recipe</u> <u>parameter "Mass Mode"</u> ).
Mary	Add Scan Chart	Add an (empty) scan chart to the section.
		Only available for scan recipes.
Phys.	Add Scan Task	Depends on the working area into which you drag the tool:
		<ul> <li>Dragging the tool to the recipe editor:         Add a scan measurement task to the         recipe.</li> </ul>
		<ul> <li>Dragging the tool to the chart:         Add a scan measurement task to the recipe. Display the data of this measurement task in the chart.     </li> </ul>
		Only available for scan recipes (see <u>recipe</u> <u>parameter "Mass Mode"</u> ).
Q	Add Total Pressure	Icon only available for QMG220.
lacksquare	Task	Depends on the working area into which you drag the tool:
		<ul> <li>Dragging the tool to the recipe editor:         Add a new total pressure measurement         task to the recipe.</li> </ul>

# QUADERA HTML Help

		Dragging the tool to the chart:     Add a total pressure measurement task to the recipe. Display the data of this measurement task in the chart.
	Add Working Area	Create a new working area in the current recipe or measurement project.
<b>~</b> _	Remove Chart Element	Delete a measuring line or a measurement task from the chart.
(*)	Remove Section	Delete the selected section.
	Remove Section Content	Delete all objects of a section, such as charts and measurement tasks etc.
	Remove Working Area	Delete the current working area.
	Split Section Bottom	Split the section in half horizontally. A new section is added to the bottom of the present contents.
	Split Section Left	Split the section in half vertically. A new section is added to the left of the present contents.
	Split Section Right	Split the section in half vertically. A new section is added to the right of the present contents.
	Split Section Top	Split the section in half horizontally. A new section is added to the top of the present contents.

# **Measurement Project Window**

The measurement project window is a subarea of the QUADERA® <u>user interface</u>.

The measurement window is used to display a measurement project and contains the following areas:

- Recipe selection,
- Working area,
- Working area selection.

# **Recipe Selection**

The recipe selection is a subarea of the measurement project window.

The recipe selection tab allows you to switch to a recipe within a measurement project.

# **Working Area**

The working area is a subarea of the measurement project window or of a recipe.

The working area is used for displaying measuring data and for editing the currently selected recipe. The recipe editor is present in every recipe and cannot be removed by the user. Additional display areas serve as containers for the related measuring data displays. The user can add several display areas to a recipe.

# **Working Area Selection**

The working area selection is a subarea of the measurement project window.

Several working areas are available for each recipe. The working area selection tabs allow you to switch between the displays.

#### **Device Status View**

The device status view is a subarea of the QUADERA® user interface.

The device status view shows the most important device parameters and states. At a glance, you can see all the important information on the status of the connected device, the measurement and the recipe. The displayed icons and parameters are predetermined and cannot be hidden. Use the icons to easily access the basic functions of the software and the device:

Icon	Description	
	Device disconnected. Click on the icon to connect the device.	
47	Device connected. Click on the icon to disconnect the device.	
<b>:</b>	Basic device settings. Click on the icon to view the basic device settings in the "Device Configuration" window, and edit as appropriate.	
	Measurement stopped. Click on the icon to start the measurement.	
•	Measurement running. Click on the icon to stop the measurement.	
Col	Filament off. Click on the icon to switch the filament on.	
	Filament on. Click on the icon to switch the filament off.	
	SEM off. Click on the icon to switch the SEM on.	
<b>22</b>	SEM on. Click on the icon to switch the SEM off.	

#### **Common SEM Voltage**

Common operating voltage of the SEM. Enter the required value or use the spin buttons. Measurement tasks will use the "Common SEM Voltage" if <<SEM-Voltage>> is selected from the dropdown list for the corresponding recipe parameter "SEM Voltage".

#### NOTE:

The "Common SEM Voltage" parameter is not available when the Faraday-Cup has been selected in the basic device settings (Symbol "Device Configuration View").

#### **All Device Status View**

The All Device Status View is a subarea of the QUADERA® user interface.

The All Device Status View shows a collection of the most important device parameters and states for all devices connected to QUADERA. At a glance, you can see all the important information on the status of the connected device, the measurement and the recipe. The displayed icons and parameters are predetermined and cannot be hidden. Use the icons, described on the Device Status View page, to easily access the basic functions of the software and the device.

The All Device Status View allows for selection of multiple devices (using CTRL or Shift key) and provides a context menu for selection of functions. The All Device Status View is most useful for viewing status when operating QUADERA in the Multiplexing mode.

Please note that the All Device Status View does not replace the Start Page as the main control. You must still use the Start Page and its Device icons to access Projects and Templates for a Device.

### **Event View**

The event view is a subarea of the QUADERA® user interface.

The event view informs you of events that have occurred for each device (the selected device on the Start page). Warnings, informations and errors are displayed in a compact way.

Events related to measurement, device and system are listed. The presentation follows the event view used by the Windows operating system. Refer to the <u>list of events</u> for a detailed description.

### **Context Menus**

### **Context Menus**

A context menu is a special menu that opens up when pressing the right mouse button. It is context sensitive and always contains commands which are related to the currently used screen area.

In QUADERA®, you may call up context menus in the following screen areas:

<u>Title bar</u>	Context menu with functions relating to the QUADERA® window.
Window title	Context menu with functions relating to the respective window in QUADERA®.
<u>Menu bar</u>	Context menu with functions relating to the menu bar settings.
Recipe Selection	Context menu used for adjusting the recipe layout (working area)
Frame of the section	Context menu used for showing and hiding the navigator.
Charts in the working area	Context menus with functions used for adjusting the chart layout.

Context menus in QUADERA®

# Calling Up a Context Menu

- 1. Position the mouse pointer in the required screen area.
- 2. Press the right mouse button.

### Context Menu "Title Bar"

Click with the right mouse button into the title bar of a window. The context menu "title bar" appears. It contains the following functions:

	Restore	Restore the default size for the selected window.
	Move	Move the window.
	Size	Change the window size.
_	Minimize	Minimize the window size.
	Maximize	Maximize the window size.
X	Close	Close the window or the application.

#### Context Menu "Menu Bar"

Click with the right mouse button into the menu bar. The context menu "Menu bar" appears. It contains the following functions:

Lock the Checkbox: Determine whether or not it is possible to change the positions of the menu

bars.

• Customize... Open a window which allows you to customize

or create menu bars, and also to configure

keyboard shortcuts.

### Context Menu "Recipe Selection"

Click with the right mouse button into the recipe selection area. The context menu "Recipe Selection" appears. It contains the following functions:

 Rename Open the dialog field "Rename selected tab" to selected tab rename the tab of the selected working area.

### Context Menu "Frame of the Section"

Click with the right mouse button into the frame of the section. The context menu "Frame of the section" appears. It contains the following functions:

Show Show or hide the data navigator.
 Navigator

• Rename Open the dialog field "Rename selected tab" to selected tab rename the tab of the selected working area.

### Context Menu "Chart"

Click with the right mouse button into a chart located in the working area. Various context menus are available, depending on the selected mouse pointer position:

- Click on the measuring data display. Context menu "Chart" appears. It contains the following functions:
  - Zoom Out
  - Reset Zoom
  - Hold
  - Legend
  - Print
  - Enable Background Subtraction
  - Enable Reference Subtraction
  - View as Partial Pressure
  - Marker (only in MID/MCD recipes)
  - <u>Display</u> (only in MID/MCD recipes)
  - Analog I/O Characteristics
- Click on the x-axis. <u>Context menu "Axis X"</u> appears.
- Click on the y-axis. Context menu "Axis Y" appears.
- Only when the legend is shown: Click on the chart legend. <u>Context menu</u> <u>"Legend"</u> appears.
- Only for trending charts in MID/MCD recipes: Click on the right y-axis. <u>Context menu "Axis Y2"</u> appears.

### Context menu "Chart"

Click on the measuring data display to open this context menu.

- Zoom Out Undo the last zoom action.
- Reset Zoom Undo all zoom actions, i.e. reset the display to the initial area.
- Hold

- Enabled (with checkmark):
   Freeze the display during a measurement (no scaling and scrolling). Measuring data are still recorded and stored. "Hold On" is automatically selected when zooming or moving the cursor.
- Disabled (no checkmark):
   Disable the hold function and resume to display the recording of data. "Hold Off" is usually applied after zooming or moving the cursor.

NOTE: There is one hold function for each

working area.

Legend

- Enabled (with checkmark): The chart legend is displayed.
- Disabled (no checkmark):
   The chart legend is not displayed.

Print

- Print this Item: Prints the chart displayed.
- Print Full Report: Prints a report based on the Print Preferences.
- Set Print Preferences: Allows selection of items to print in the Full Report.
- Print Preview: Provides a preview of what will be printed in the Full Report.
- Enable Background Subtraction

Allows Background Subtraction to be enabled and disabled.

 Enable Reference Subtraction Allows Reference Subtraction to be enabled and disabled in a Reference Subtraction measurement project.

 View as Partial Pressure Allows viewing MID data as Partial Pressure (or Amps).

Marker

Only available for trending charts in MID/MCD recipes:

- Enabled (with checkmark):
   Displays the individual measuring points and the connecting lines.
- Disabled (no checkmark):
   Displays the connecting lines of the measuring points.

Display

Only available for MID/MCD recipes.

Switch the representation of the chart:

- Trend:
  - Continuously display the measuring data as a function of the time (in the selected section, see data navigator).
- Bar:

Display the measuring data in a bar graph at the time specified by the cursor, see data navigator.

• Table:

Display the measuring data in a table at the time specified by the cursor, see <u>data</u> navigator.

Analog I/O

Allows assignment of a characteristic to an

Characteristics Analog I/O (if available).

### Context menu "Axis X"

Click on the x-axis to open this context menu. It is used to switch the presentation of the x-axis.

Fixed Range of the axis is fixed

Only in scan recipes

Automatic
 Range of the axis is adjusted to the measured

values

Only in scan recipes

• Time Absolute Display the absolute time (date, time)

Only in MID/MCD recipes

Time Relative Display the relative time (measuring time)

Only in MID/MCD recipes

### Context menu "Axis Y"

Click on the y-axis to open this context menu. It is used to switch the presentation of the y-axis.

Linear axis scaling

Logarithmic Logarithmic axis scalingFixed Range of the axis is fixed

Automatic

Range of the axis is adjusted to the measured

values

### Context menu "Axis Y2"

This context menu is available only in MID/MCD recipes, and at least one measurement task is assigned to the second y-axis (via context menu "Legend"). Click on the right y-axis to open this context menu. It is used to switch the presentation of this axis.

Linear axis scaling

Logarithmic Logarithmic axis scaling
 Fixed Range of the axis is fixed

Automatic
 Range of the axis is adjusted to the measured

values

### Context menu "Legend"

This context menu is available only when the chart legend is shown (via context menu "Chart"). Click on a measurement task in the legend to open this context menu.

• Chart Element Indicates the measurement task related to the

Axis Y1

The measuring data display of the indicated measurement task uses the left y-axis. You can define the y-axis for each measurement task, i.e. if the left or right y-axis is used for this task.

Only for MID/MCD recipes

Axis Y2

The measuring data display of the indicated measurement task uses the right y-axis. Context menu "Axis Y2" becomes available. You can define the y-axis for each measurement task, i.e. if the left or right y-axis is used for this task.

Only for MID/MCD recipes

• Color...

Opens the <u>"Color" dialog</u> to select the color for the chart display of the measurement task (curve color).

Note that you can also define the <u>line</u> thickness of the curve.

### Context Menu "Docker Window"

#### NOTE:

This context menu is only available for the docker windows (Toolbox, Device Status View, All Device Status View, Event View), but not for the measurement project window and the start page.

Click with the right mouse button into the docker window title. The context menu "Docker Window" appears. It contains the following functions:

Dockable

Checkbox: Specify if the selected docker window is dockable or not.

No:

The behavior of the docker window is the same as known from a normal window. It appears in the <u>window list</u>, in the bottom part of the Window menu.

Yes:

When you move the docker window various anchoring points are displayed on the user interface. The "Floating" property is automatically assigned to the docker window if you do not move it on an anchoring point. Note that you can move the toolbox only to the displayed anchoring points.

• Hide

Checkbox: Specify if the selected docker window is shown or hidden. Use the View menu to show a hidden window.

Floating

Checkbox: Specify if the selected docker window can be moved freely (even outside of the window of the related application).

### Note:

- "Floating" docker windows are always "Dockable".
- The "Floating" property can not be assigned to the toolbox.
- Auto Hide

Checkbox: Specify if the auto-hide function is enabled for the selected docker window, i.e. the corresponding docker window will be automatically hidden and shown if needed.

## **Capturing Screenshots of the User Interface**

As a written documentation for your measurement projects you can capture and print out screens of the QUADERA® user interface. Proceed as follows:

- 1. Capture the screen. The screenshot is copied into the Windows clipboard:
  - Full screen capture: press the key combination "CTRL+Print",
  - Active window capture: press the key combination "CTRL+ALT+Print".
- 2. Open a suited image editor, e.g. Microsoft Paint (Windows start menu > Programs > Accessories > Paint).
- 3. Paste the screenshot from the Windows clipboard into the image editor, e.g. press the key combination "CTRL+V".
  - 4. Use the image editor to print out the screenshot.

#### NOTE:

Various screen capture tools are available as freeware, shareware, and by purchasing. In general, these tools provide enhanced screen capture features compared to the procedure described above.

# **Getting Started**

## **Starting QUADERA®**

You can start QUADERA® from the Windows Start menu or from the desktop.

### Windows Start menu

- 1. Click the Windows **Start** button and select the **All Programs** entry.
- 2. Select the QUADERA program group and click the QUADERA entry.

### Desktop

You can start QUADERA® from the desktop if a shortcut has been created for the desktop during installation.

1. Double-click the **QUADERA** shortcut symbol on your desktop.

After starting QUADERA®, the start page is displayed.

## **Start Page**

The Start Page selection (File or a Device) determines what is displayed within the views of QUADERA® (e.g. Measurement Projects, Event View, Device Status View, title bars, etc.). For example, select a device on the start page to see its Event View.

After starting QUADERA®, the start page is displayed. Here you can perform one of the following actions:

- Open existing measurement projects (\*.qmp files) and work with them:
  - Click on the File icon. All measurement projects that have been worked on recently are shown in a list. Select the required project and open it with OK or by double-clicking it.
  - Click the More... button to open a measurement project that is not present in the list.
- Selecting templates to start new measurements:
  - Click on the icon for the required device (Simulator or real device).
  - If you want to start a new measurement: Click on the "Templates" bar and select the desired template (measurement project templates \*.qmt in the "Templates" list).
  - If you want to calibrate the device:

    Click on the "Calibration and Tuning" bar and select the desired template

    (calibration templates \*.gmt in the "Calibration and Tuning" list).
  - Only QMG220: If you want to start a new RGA application (Residual Gas Analysis):
     Click on the "RGA Application" bar and select the desired template (measurement project templates \*.gmt in the "RGA Application" list).

If the start page is not displayed, you can call it up as follows:

- In the View menu, click Show Start Page. The start page is displayed.
- Only if the start page is already open: In the **Window** menu, click the respective item in the list of open windows.

### NOTE:

Continuing the measurement using an existing measurement project is not possible.

# **Example of a Measurement**

## Introduction

The goal of this sample measurement is to analyze the composition of air. For this, we do not perform a real measurement in vacuum. Instead, we are going to use the simulation mode of QUADERA® and the stored simulation data which represent a typical measurement of air with a Faraday detector. Except for small details, the <u>course of a measurement</u> is the same for all mass spectrometers.

### Course of a Measurement - Scan

#### NOTE:

For software training and in order to practice the measurement runs we recommend that QUADERA® be used in the simulation mode.

The scan measurement type (ion current as a function of m/e) is suitable for obtaining an overview of all present gases.

- 1. Open the start page: In the View menu, click Show Start Page.
- 2. Click on the icon for the required device.
- 3. Create a new measurement project: In the "Templates" list, double-click e.g. **Airdemo Scan Analog.qmt**. This way you create a new measurement project based on the selected template.

Please note: The file extension for templates is \*.gmt

- 4. The new measurement project window appears. The working area displays the scan project.
  - Edit the recipe (if necessary): Click the Edit tab.
  - Display the measuring data: Click the **Measure** tab.

#### NOTE:

You can start the measurement regardless whether the recipe editor or the working area has been selected.

- 5. Start the measurement: In the device status view, click on the "Start" icon. The connection to the device is automatically established. The device now receives the parameters for the current measurement task. You can adjust the chart layout while the measurement is running.
- 6. Stop the measurement: In the device status view, click on the "Stop" icon.
- 7. Close and save the measurement project. In the **File** menu, click **Close**. You are requested if you want to save the measurement project. QUADERA® suggests an automatically generated file name that is based on date/time of the measurement and the used template.
  - Yes: the "Save As" window used for saving measuring data opens up. Select a suitable name and path and then click **Save**. The measurement project will be saved and closed.
    - Please note: The file extension for measurement projects is \*.qmp
  - No: the measurement project will be closed without saving the data.
  - Cancel: the action is cancelled. You will return to the measurement project without saving the data.

### **Course of a Measurement - MID**

#### NOTE:

For software training and in order to practice the measurement runs we recommend that QUADERA® be used in the <u>simulation mode</u>.

The MID measurement type (Multiple Ion Detection) is suitable for observing changes of several gases with time.

- 1. Open the start page: In the View menu, click Show Start Page.
- 2. Click on the icon for the required device.
- 3. Create a new measurement project: In the "Templates" list, double-click e.g. **Airdemo MI D.qmt**. This way you create a new measurement project based on the selected template.

Please note: The file extension for templates is \*.gmt

- 4. The new measurement project window appears. The working area displays the MID project.
  - Edit the recipe (if necessary): Click the Edit tab.
  - Display the measuring data: Click the **Measure** tab.

#### NOTE:

You can start the measurement regardless whether the recipe editor or the working area has been selected.

- 5. Start the measurement: In the device status view, click on the "Start" icon. The connection to the device is automatically established. The device now receives the parameters for the current measurement task. You can adjust the chart layout while the measurement is running.
  - 6. Stop the measurement: In the device status view, click on the "Stop" icon.
  - 7. Close and save the measurement project. In the **File** menu, click **Close**. You are requested if you want to save the measurement project. QUADERA® suggests an automatically generated file name that is based on date/time of the measurement and the used template.
  - Yes: the "Save As" window used for saving measuring data opens up. Select a suitable name and path and then click **Save**. The measurement project will be closed and saved.
    - Please note: The file extension for measurement projects is \*.qmp
  - No: the measurement project will be closed without saving the data.
  - Cancel: the action is cancelled. You will return to the measurement project without saving the data.

## **Chart Display**

In the working area selection, click the **Measure** tab (or the tab which corresponds to the required working area). The measuring data of the project are displayed in the section (chart display):

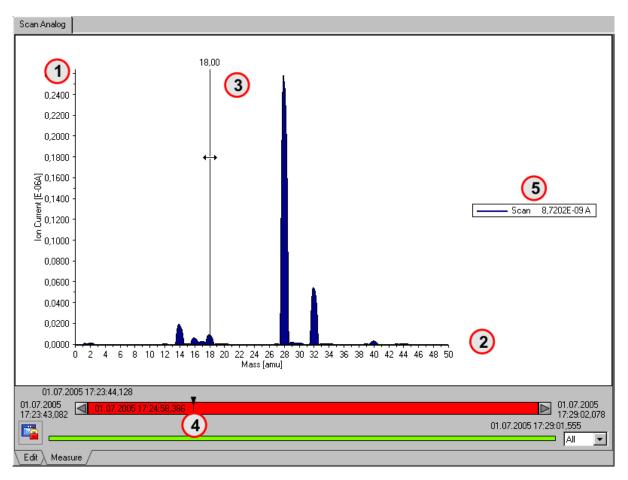


Chart display (example)

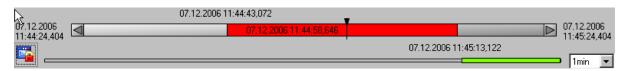
- 1 Y-axis
- 2 X-axis
- 3 Cursor, indicates the x-axis position (mass)
- 4 Data navigator
- 5 Legend (measuring value at the cursor position)
  - You can navigate in the measuring data by means of the <u>data navigator</u> or by pulling the cursor (mouse pointer is displayed as a double arrow).
  - The context menus for the chart gives you access to additional functions.
  - Use the <u>tools</u> "Add Chart Element" and "Remove Chart Element" to add and delete existing measurement tasks to and from the chart, respectively.

### **Data Navigator**

### **Data Navigator**

You can show and hide the data navigator by means of the context menu "frame of the section".

The data navigator is located below the measurement display. It allows you to scroll through the measuring data along the time axis. This is possible while a measurement is running and also for stored measuring data. If a measurement is running, this will automatically freeze the display (hold mode). You can exit the hold mode with the <a href="Hold">Hold</a> Off function, e.g. by clicking on the "Hold Mode" icon.



Data navigator

The data navigator contains the following parts:

- The lower navigator bar comprises the entire measurement period. Use the dropdown list to the right of the bar to select the required period. This period will be represented by a green scroll bar.
  - Time period ("1 min"..."4 weeks"): The measuring values of the selected time period can be displayed.
  - All: All measuring values can be displayed.
- The upper navigator bar comprises the time period that has been selected in the lower navigator bar (green bar). The range limits are displayed at the left and right end of the bar.
- The red scroll bar inside of the upper navigator bar comprises a time period whose range limits are displayed at the upper left and lower right end of the bar (it covers 1 minute in the above example "Data navigator").
- The cursor in the upper navigator bar (vertical line) is used to determine which point of time is to be displayed in the chart. This point of time is displayed next to the cursor.

### Icon "Hold Mode"



"Hold On": the display is frozen (hold mode is on).

Click on the icon to exit the hold mode.



"Hold Off": the display is updated (hold mode is off).

Click on the icon to activate the hold mode.

### Using the data navigator

The data navigator allows you to quickly access the entire measurement period. You can easily move the time window displayed in the chart across the entire navigation area. The measurement displays in different sections are synchronized. Most measurements cover a rather restricted period of time. For this reason, the lower navigator bar is only rarely used. The two-bar design is only required for improved navigation when handling very large amounts of data.

- Data navigator and zooming
- <u>Data navigator in scan measurements</u>
- <u>Data navigator in MID/MCD measurements</u>

# **Data Navigator and Zooming**

#### Scan measurements

In a scan measurement, the data navigator refers to the chronological order of the individual scans (measuring cycles). This is useful when navigating between the individual measuring cycles. The <u>zoom function</u> applies to the scan displayed in the chart (intensity as a function of the mass) and is independent of the data navigator. The selected magnification is maintained if you select another measurement cycle or change the time period with the data navigator.

### MID/MCD measurements "Trend"

In the "Trend" view, the data navigator displays the time period of the zoomed detail. The red scroll bar in the upper data navigator is synchronized with the <u>zoom function</u> of the x-axis (time).

The selected magnification is maintained if you move the time period displayed in the chart with the data navigator, or if you change the time period.

### MID/MCD measurements "Bar"

In the "Bar" view, the cursor position in the data navigator specifies the point in time for which the measuring data are displayed. In a bar graph, the <u>zoom function</u> is independent of the data navigator and it applies to the intensity (y-axis) only. The selected magnification is maintained if you move the time period displayed in the chart with the data navigator, or if you change the time period.

### MID/MCD measurements "Table"

There is no zoom function available in the "Table" view. The data in the table represent the measured values at the time that is indicated by the cursor position in the data navigator.

### 32,00 0,2600 0,2400 0,2200 0,2000 0,1800 0,1600 0,1400 0,1200 0,1000 5,0418E-08 A Scan 0,0800 0,0600 0,0400 0,0200 0,0000 10 25 20 30 Mass [amu] 01.07.2005 17:27:33,639 3 01.07.2005 01.07.2005 17:27:33,639 17:28:33,639 01.07.2005 17:28:33.639 1min

## **Data Navigator in Scan Measurements**

Chart display: Example of a scan measurement

The chart displays a scan (intensity as a function of the mass) at a point in time which is specified by the cursor position in the data navigator (item 3 in the above figure). It is only possible to display the scans in the time period specified by the red scroll bar in the upper navigator bar.

The measuring values displayed in the chart are determined by the cursor positions in the data navigator and in the chart. The following rules apply:

- The cursor in the upper navigator bar (item 3) determines which scan is to be displayed in the chart, i.e. the point in time of a scan within the entire measurement period (measurement cycle).
- The cursor in the chart (item 1) determines the mass (x-axis) in the displayed scan for which the measuring values are listed (item 2).

## **Data Navigator in MID/MCD Measurements**

Select the required chart view using the "Diagram" context menu.

### "Trend" view

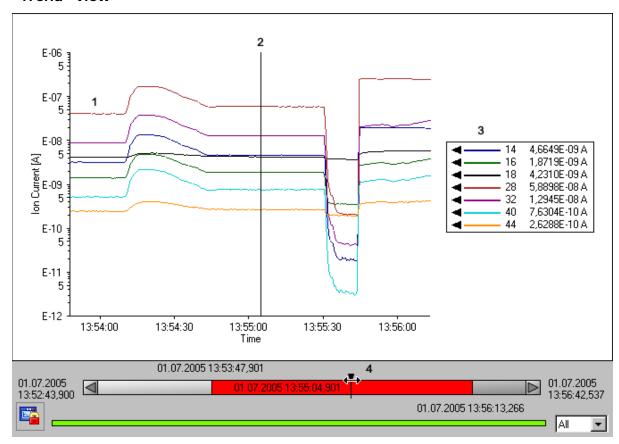


Chart display: Example of a sample measurement (trend)

The measurement data (item 1 in the above figure) are displayed as a function of the time. The chart covers the period of time which is specified by the red scroll bar in the upper navigator bar. The displayed measuring values (item 3) are specified by the cursor position. Please note that the cursor in the red scroll bar (item 4) and the one in the chart (item 2) are synchronized.

### "Bar" view

The measuring data are displayed as a bar graph for the point in time specified by the cursor position in the data navigator. The measuring data can only be displayed within the period of time specified by the red scroll bar in the upper navigator bar.

### "Table" view

The measuring data are listed as a table for the point in time specified by the cursor position in the data navigator. The measuring data can only be displayed within the period of time specified by the red scroll bar in the upper navigator bar. Please note that

the average and the maximum values are still based on the entire time of the measurement.

# **Exiting QUADERA®**

Use one of the following methods to exit QUADERA®:

- In the **File** menu, click **Exit**.
- Press **ALT+F4** (standard method for exiting the currently active Windows application).
- Click the Close symbol **X** in the upper right corner of the QUADERA® window.
- Call up the context menu for the title bar of the QUADERA® window and click **Close**.

# **Opening and Managing Measurement Data**

# **Opening an Existing Measurement Project**

- 1. In the **File** menu, click **Open**.
- 2. Select the directory, the file name and the file type for the required measurement project.
- 3. Click Open.

You may also open an existing measurement project via the **Start page**.

### NOTE:

Continuing the measurement in an existing measurement project that is already saved is not possible. The relevant icons and menu commands are not available.

# **Recently Used Files**

Proceed as follows to open a recently used file:

- 1. The most recently used files are listed in the lower part of the **File** menu. Click the **More...** button to open a measurement project that is not present in the list.
- 2. Click the required file in order to open it.

You may also open a recently used file via the **Start page**.

## **Exporting a Measurement Project**

#### NOTE:

If you have not selected a section of a Measurement Project then the Export submenu item is disabled.

### **Exporting**

Proceed as follows to export the data of an open measurement project:

- 1. Select the required section.
- 2. In the **File** menu, click **Export**.
- 3. Select the required data format in the submenu:
  - **ASCII** will export the displayed data in the text-only format. You may open and further process these data in any spreadsheet program (e.g. Excel).
- 4. The "Export Options" window used for selecting measuring data opens up.
  - a. Select the required measurement tasks in the "Measure Tasks" area.
    - b. Select the required data in the "Data Range" area.
      - "All" exports all data of the measurement project,
      - "Selection" exports only the displayed data in the selected section (scan chart, MID chart etc.),
      - "Cycles" exports the selected cycles of the measurement project.
- 5. Click **OK**. The "ASCII-Export data as" window used for exporting measuring data opens up. Select a suitable name and path and then click **Save**. The measurement project will be exported.

Delimiters, the date and time format, and decimal separators (period and comma) are country specific. These settings can be adjusted in the operating system: Windows Start menu > Control Panel > Date, Time, Language, and Regional Options. The settings for the operating system will also be used by QUADERA®.

## Closing a Measurement Project

- 1. Select the required measurement project window.
- 2. In the File menu, click Close.

or

2. Click the Close symbol x in the upper right corner of the measurement project window.

### Saving a new measurement project

When closing a new measurement project you are requested to save the measurement project. QUADERA® suggests an automatically generated file name that is based on date/time of the measurement and the template in use.

- Yes: the "Save As" window used for saving measuring data opens up. Select a suitable name and path and then click **Save**. The measurement project will be closed and saved.
  - Please note: The file extension for measurement projects is \*.qmp
- No: the measurement project will be closed without saving the data.
- Cancel: the action is cancelled. You will return to the measurement project without saving the data.

## Changing a File Location

In QUADERA®, you can specify the path (file location) for various file types created by the user:

- Templates: Measurement project templates,
- Calibration files: Files containing calibration templates,
- · Data files: Files containing measurement projects,
- Exported files: Files containing exported projects.
- Scripting files: Files containing scripting code (Add-ins).

Proceed as follows to change the corresponding paths:

- 1. In the **Tools** menu, click **Options...**. The "Options" window opens up.
- 2. Click the File Locations tab.
- 3. Select the desired file type.
- 4. Click Modify.
- 5. The "Browse For Folder" window opens up. Select the desired path and then click **OK**.
- 6. In the "Options" window, click **OK**.

### NOTE:

Click "Default" to reset the paths for all file types to the default settings.

# **Changing the Display of Measurement Projects**

# **Adjusting the Section**

You can adjust the display of measuring data in the section, even while a measurement is running. Proceed as follows:

- 1. Click the section with the right mouse button. The related context menu opens up.
  - 2. Click the required function.

# **Zooming in Charts**

#### Selection of the zoom area

Use the mouse pointer (displayed as crosshairs in a <u>chart</u>) to mark a rectangle across the required area:

- 1. Position the crosshairs in one corner of the required rectangle.
- 2. Press the left mouse button and keep it pressed.
- 3. Move the cursor to the opposite corner of the rectangle. The zoom area is indicated by a dashed rectangle.
- 4. Release the left mouse button. The marked area is zoomed in.

### NOTE:

For sample measurements, the <u>data navigator</u> displays the time period of the zoomed area of the x-axis (time axis).

### Resetting the zoomed area

- 1. Call up the related context menu.
- 2. Click Zoom out or Reset Zoom.

# **Selecting Curve Colors in Charts**

You can select curve colors in charts.

### Proceed as follows:

- 1. Click with the right mouse button into the measuring data legend of the section. The corresponding <u>context menu</u> opens.
- 2. Click on **Color...** The "Color" dialog opens.
- 3. Select the required curve color.
  - Click one of the available basic colors, or
  - Click one of the color fields that has already been defined by you, or
  - Click [Define Custom Colors>>]. A continuous color palette appears and allows you to select a color.
- 4. Click [OK] to confirm the selection.

For a more detailed description of the "Color" dialog box, please refer to the Windows operating system help.

# **Defining the Line Thickness in Charts**

You can change the line thickness of curves in charts.

### Proceed as follows:

- 1. In the **Tools** menu, click **Options...**. The "Options" dialog opens.
- 2. Click the **Display** tab.
- 3. Enable the "Smooth Chart Lines" checkbox to smooth the displayed lines in charts.
- 4. Use the spin buttons to increase and decrease the line thickness.

The settings are applied to the charts for all measurement projects.

# **Splitting Up the Working Area**

You can split up the working area into several sections, i.e. you can add new sections.

### Toolbox

Proceed as follows:

- 1. Select the required working area.
- 2. Open the corresponding toolbox.
- 3. Drag the required tool ("Split") onto the working area (drag&drop). The section is split up according to the selected tool.

# **Deleting a Section**

### NOTE:

Measurement data remain stored when a section is deleted.

You can remove sections of the working area, i.e. you can delete a section.

### Toolbox

Proceed as follows:

- 1. Open the corresponding toolbox.
- 2. Drag the **Remove Section** tool onto the required section (drag&drop).
- 3. You are asked to confirm the deletion of the section. Click **OK**.

The section is deleted and the working area is simplified.

# **Creating a New Working Area**

You can create a new working area in a measurement project. This allows you to display the measurement tasks of a measurement project in different ways according to your requirements (e.g. different combinations of measurement tasks, or the representation as a curve and a bar graph).

#### Toolbox

Proceed as follows:

- 1. Select the required measurement project.
- 2. Open the corresponding <u>toolbox</u>.
- 3. Drag the **Add Working Area** tool onto the working area (drag&drop). A new tab labeled "New WorkingArea" appears in the working area selection, and the new working area is displayed.
- 4. Use the context menu "Frame of the section" to rename the new working area as desired.

# **Deleting a Working Area**

### NOTE:

Measurement data remain stored when a working area is deleted.

You can delete working areas in a measurement project.

### Toolbox

Proceed as follows:

- 1. Select the required measurement project.
- 2. Open the corresponding toolbox.
- 3. Drag the **Remove Working Area** tool onto the working area (drag&drop).
- 4. You are asked to confirm the deletion of the working area. Click **OK**.

The working area is deleted.

# Freezing the Display

You can freeze the display while a measurement is running. This will allow you e.g. to scroll through a measurement or to zoom an area.

### Proceed as follows:

- 1. Click on the measuring data display in the section with the right mouse button. The related context menu opens up.
  - 2. Click **Hold**:
  - The checkmark indicates that the function is enabled, i.e. the display is now frozen.
  - The function is disabled if the checkmark is not shown.

or

1. Click on the <u>"Hold mode" icon</u> in the data navigator. Note that the icon is only displayed when the data navigator is shown.

### NOTE:

If you are zooming an area or moving the cursor, the "Hold" function will be switched on automatically, i.e. the display will freeze.

## **Managing and Arranging Windows**

### **Displaying Windows**

QUADERA® can manage several windows at a time. Individual windows can be handled as usual under the Windows operating system (close, move, resize, etc.). You may also use the title bar context menu for the respective window. In addition, the following options are available:

- Show all windows
- Close all windows
- Switch between windows
- Arrange icons

### Showing all windows:

- In the **Window** menu, click **Cascade**. This will arrange all open windows in an overlapping manner.
- In the **Window** menu, click **Tile Horizontally**. This will arrange all open windows as horizontal tiles (one below the other).
- In the **Window** menu, click **Tile Vertically**. This will arrange all open windows as vertical tiles (side by side).
- In the **Window** menu, click **Minimize All Windows**. This will minimize all open windows.

### Closing all windows:

• In the **Window** menu, click **Close All Windows**. This will close all open windows.

### Switching between windows:

- 1. Open the **Window** menu. A list of all open measurement projects is displayed at the bottom of the pulldown menu.
- 2. Click the required measurement project in order to move the related window to the front.

## QUADERA HTML Help

When switching to another measurement project, the device status display is always updated. This means that the status of the device belonging to the current measurement project is displayed.

## **Arranging icons:**

• In the Window menu, click Arrange Icons. This will arrange all icons.

# **Showing and Hiding Docker Windows**

You can show and hide <u>docker windows</u> in the **View** menu.

- Enable the docker window if you want it to be shown,
- Disable the docker window if you want it to be hidden.

### **Event view**

In the View menu, click the Event View element to show and hide the event view.

#### **Device status**

In the View menu, click the **Device Status** element to show and hide the <u>device status</u>.

#### Toolbox

In the View menu, click the Toolbox element to show and hide the toolbox.

# **Calling Device Specific Functions**

# **Configuring the Device Connection**

The device connection is automatically configured. One simulator per Device type is present (if licensed); other mass spectrometers can be added using 'Search' in 'Device>>Device Setup'.

## Starting and Stopping the Measurement

component is to be switched on or not.

#### NOTE:

New or modified parameters for the measurement task are accepted from the device only after the measurement has been restarted. Ion source parameters affect the device immediately, i.e. as soon as the device is connected with QUADERA®.

### Starting the measurement

- In the device status view, check that the filament and SEM are on. The
  corresponding icons and tooltips indicate the current status. If required, switch
  the filament and the SEM on.
  When the filament and the SEM are switched off and you want to start the
  measurement a requester appears automatically. It gueries if the corresponding
- 2. In the **Device** menu, click **Run**. The connection to the device is automatically established and then the current recipe is started. The checkbox indicates that the measurement is running (checkmark).

or

2. In the device status view, click the "Start" icon \_\_\_\_\_\_. The connection to the device is automatically established and then the current recipe is started. The "Start" icon appears in gray thus indicating a running measurement. The "Stop" icon becomes available.

### Stopping the measurement

1. In the **Device** menu, click **Run**. The measurement is being stopped. The checkbox indicates that the measurement has been stopped (no checkmark).

or

1. In the device status view, click the "Stop" icon \_\_\_\_\_. The measurement is being stopped. The "Stop" icon appears in gray thus indicating that the measurement is stopped. The "Start" icon becomes available.

# **Disconnecting From the Device**

### Disconnecting

1. In the **Device** menu, click **Connect**. The checkbox indicates that the device is no longer connected (no checkmark).

or

1. In the device status view, click the "Connected" icon

After the connection
has been cut the icon toggles to the "Disconnected" icon.

### NOTE:

A requester appears if you disconnect the device while the measurement is running:

- Click "Yes" if you want to disconnect the device. The measurement will be stopped.
- Click "No", if you want to continue the measurement. The device will not be disconnected.

# **Connecting With the Device**

#### NOTE:

New or modified parameters for the measurement task are accepted from the device only after the measurement has been restarted. Ion source parameters affect the device immediately, i.e. as soon as the device is connected with QUADERA®.

### **Start Page**

• Select the desired device. You can choose between a real device and a simulator.

### Connecting

- In the **Device** menu, click **Connect**. The checkbox indicates that the device is connected (checkmark), or

### **Simulation Mode**

QUADERA® allows you to simulate the operation of a mass spectrometer. This doesn't mean that a simulation is being performed in the real device; instead, a simulation software is used. By default, the simulation software is installed together with QUADERA®. The simulator is running on the same PC as QUADERA®. The local simulation mode is e.g. helpful for getting familiar with the software.

To use the simulator, select it on the 'Start Page' and use it as you would a real device.

#### NOTE:

The simulation in the real device is defined via the basic device settings of the device status view ("Device Configuration View" icon). In contrast, using the simulation software (local simulation on the PC) does not require a real device.

### Calibration

## **Calibration Projects**

In QUADERA®, devices are calibrated by using calibration projects, which are based on normal measurement projects. Calibration projects are called via the start page.

A calibration project contains the usual views of a measurement project:

- One recipe,
- Working areas for operation and visualization.

You can modify recipe parameters directly in the recipe. The parameters that are relevant for the calibration project are linked to editing fields in the working area. Thus, you can change these parameters directly in the working area.

QUADERA® provides basic templates for each calibration project, such as gas specific calibration and background determination. These templates are intended to create user specific calibration project templates, for ab initio calibration projects.

Saving the measurement data of a calibration procedure is usually not required. However, saving the calibration project as a template may be useful for future applications (menu <a href="File">File</a> > Save as Template...). Example: creating GSC measurement projects.

#### NOTE:

For a written documentation of your calibration projects you can <u>capture</u> <u>screens</u> of the QUADERA® user interface.

## **Tuning the Ion Source**

## **Tuning the Ion Source**

Consider one or two peaks of a scan-analog measurement to tune the ion source (ion source optimization). Use the <u>recipe editor</u> to change the <u>recipe parameters</u> defined in the calibration project for the ion source. Typically, one or more masses are scanned.

The calibration project allows you to optimize the performance of the ion source. The scans will be recorded when you start the calibration project. The currently set <u>ion</u> <u>source parameters</u> are used. They are displayed in the working area. Tune the ion source while the measurement is running; optimize the peak shape and intensity by changing the ion source parameters. Changed parameters are forwarded from the calibration project to the device and accepted instantly.

## **Optimizing the Ion Source**

- 1. Open the start page: In the **View** menu, click **Show Start Page**.
- 2. Click on the icon for the required device.
- 3. Create a new calibration project: In the "Calibration and Tuning" list, double-click **Ion Source Tuning.qmt**. This way you create a new calibration project based on the selected template.
- 4. The new measurement project window appears. The working area displays the calibration project.
  - Edit the recipe according to your needs (if necessary): Click the corresponding tab in the working area selection.
  - Display the measuring data: Click the corresponding tab in the working area selection.

#### NOTE:

You can start the measurement regardless whether the recipe editor or the working area has been selected.

- 5. Start the measurement: In the device status view, click on the "Start" icon. The connection to the device is automatically established. The device now receives the parameters for the current measurement task. You can adjust the chart layout while the measurement is running.
- 6. Optimize the peak shape and intensity: Change the ion source parameters in the section of the calibration project during the measurement ("Ion Source" editor). Changed parameters are accepted by the device instantly.

You will find the procedures to optimize the ion source potentials for the QMG700 with QMA400/410/430 in the operating instructions BG 805983 BD/E.

Procedures to optimize the specific ion source types for the QMG220:

- Crossbeam Ion Source
- Grid Ion Source
- SPM Ion Source
- Open High Sensitivity Ion Source
- Gastight High Sensitivity Ion Source
- 7. Stop the measurement: In the device status view, click on the "Stop" icon.
- 8. Close and save the measurement project. In the **File** menu, click **Close**. You are requested if you want to save the measurement project. QUADERA® suggests an automatically generated file name that is based on date/time of the measurement and the used template.
  - Yes: the "Save As" window used for saving measuring data opens up. Select a suitable name and path and then click Save. The measurement project will be saved and closed.
    - Please note: The file extension for measurement projects is \*.qmp
  - No (recommended option): the measurement project will be closed without saving the data.

• Cancel: the action is cancelled. You will return to the measurement project without saving the data.

NOTE: The filament Ion Source can be degassed from the  $\underline{\mbox{Device Configuration}}$  window.

### **Ion Source Parameters**

The "Ion Source" editor in the calibration project displays the parameters for tuning the ion source. Modify the parameters directly in this editor. The device applies modified parameters instantly.

- Ion source parameters for QMG220
- Ion source parameters for QMG700

A separate parameter set is stored for each ion source type and filament. The QMG220 additionally provides 4 parameter sets per ion source type, containing ion source voltages ("Active Set").

Image of "Ion Source" editor (example)

### Ion source parameters for QMG220

Parameter		Range	Description
•	Ion Source Type	(not editable)	Use the "Device Configuration" window to select the ion source type.
•	Filament Number	Dropdown list	Filament selection. The number of available filaments depends on the ion source type.
•	Active Set	Dropdown list	Select the ion source voltages parameter set, which contains each one data set for the various filament configurations.
•	Emission	Number > 0	Filament emission current.
	Current		This parameter is applied to the filament that is selected under "Filament Number".
•	Protection Current	Number > 0	Maximum filament current, used to protect the filament.
			This parameter is applied to the filament that is selected under "Filament Number".
•	RF-Polarity	Dropdown list	Switch the polarity of the rod system for separating ions by the m/e-ratio.
•	Ion	Any number	Ion source voltages.
•	Reference Cathode Focus		These parameters are applied to the filament and the ion source type that is selected under "Filament Number" and "Ion Source Type", respectively. The

Field Axis

 Extraction
 Inner Deflection

 Field Axis

 available parameters depend on the used ion source. For detailed information, please refer to the operating instructions of the QMG and the used ion source.

 Outer Deflection
 Procedures to optimize the specific ion source types:

WehneltCrossbeam Ion SourceGrid Ion Source

• SPM Ion Source

• Open High Sensitivity Ion Source

 Gastight High Sensitivity Ion Source

## Ion source parameters for QMG700

Parameter		Range	Description
•	Ion Source Type	(not editable)	Use the "Device Configuration" window to select the ion source type.
•	Filament Number	Dropdown list	Filament selection. The number of available filaments depends on the ion source type.
•	Emission	Number > 0	Filament emission current.
	Current		This parameter is applied to the filament that is selected under "Filament Number".
•	<ul> <li>Filament         Protection         Current     </li> </ul>	Number > 0	Maximum filament current, used to protect the filament.
			This parameter is applied to the filament that is selected under "Filament Number".
•	Ion Reference	Any number	Ion source voltages.
•	Cathode		These parameters are applied to the filament and the ion source type that is
•	Focus		selected under "Filament Number" and
•	Field Axis		"Ion Source Type", respectively. The available parameters depend on the
•	Extraction		used ion source. For detailed
•	Inner Deflection		information, please refer to the operating instructions of the QMG and the used ion source.
•	Outer Deflection		You will find the procedures to optimize the ion source potentials for the QMG700 with QMA400/410/430 in the

• Wehnelt

operating instructions BG 805983 BD/E.

Ion Source Editor			
Ion Source Type	Crossbeam		
Active Set	Set1		
Emission Current	1,00		
Filament Number	No1		
Protection Current	4,40		
RF-Polarity	pos		
Ion Reference	105,00		
Cathode	0,00		
Focus	-6,00		
Field Axis	-7,00		
Extraction	-50,00		

#### **Crossbeam Ion Source**

This topic applies to the QMG220.

Proceed as follows to optimize the crossbeam ion source:

1. Select the filament and operate it with 1 mA emission current for approximately half an hour. The message "Emission Error" appears repeatedly: start with reduced emission current and increase it slowly.

### Default settings:

•	Emission Current:	1 mA
•	Protection Current:	4.0 A
•	RF-Polarity:	pos
•	Ion Reference:	150 V
•	Cathode:	-70 V
•	Focus:	-5 V
•	Field Axis:	-10 V
•	Extract:	-50 V

- 3. Wait until the pressure reaches  $< 10^{-7}$  mbar and the residual gas spectrum remains stable.
- 4. Introduce a test gas, such as air, into the recipient for a pressure of 10-6 mbar. Otherwise, use the residual gas to perform the optimization procedure.
- 5. Repeatedly record spectra of the relevant peaks (e.g. 25...34 m/e). Observe intensity, resolution, and peak shape.
- 6. Optimize the ion source voltages:
  - a. Check which "RF-Polarity" ("pos" or "neg") results in the better peak shape and select this polarity.
  - b. Optimize "Cathode" for best sensitivity.
  - c. Adjust "Field Axis" for useful resolution and peak shape.

d. Optimize "Extract" and "Focus" alternately for maximum peak height.

#### **Grid Ion Source**

This topic applies to the QMG220.

Proceed as follows to optimize the grid ion source:

1. Select the filament and operate it with 2 mA emission current for approximately half an hour. The message "Emission Error" appears repeatedly: start with reduced emission current and increase it slowly.

### Default settings:

•	Emission Current:	2 mA
•	Protection Current:	4.0 A
•	RF-Polarity:	pos
•	Ion Reference:	150 V
•	Cathode:	-90 V
•	Field Axis:	-12 V

Vary the "Field Axis" potential to optimize sensitivity, peak shape, and resolution.

- 3. Wait until the pressure reaches  $< 10^{-8}$  mbar and the residual gas spectrum remains stable.
- 4. Repeatedly record spectra of the relevant peaks (e.g. 25...34 m/e). Observe intensity, resolution, and peak shape.
- 5. Optimize the ion source voltages:
  - a. Check which "RF-Polarity" ("pos" or "neg") results in the better peak shape and select this polarity.
  - b. Optimize "Cathode" for best sensitivity.
  - c. Adjust "Field Axis" for useful resolution and peak shape.

### **SPM Ion Source**

This topic applies to the QMG220.

Proceed as follows to optimize the SPM ion source:

- 1. Select the filament and operate it with 1 mA emission current for approximately half an hour. The message "Emission Error" appears repeatedly: start with reduced emission current and increase it slowly.
- 2. Introduce a process gas, such as argon, into the process chamber for a pressure of  $10^{-3}...10^{-2}$  mbar.
- 3. Repeatedly record spectra of the relevant peaks (e.g. argon 32...41 m/e). Observe intensity, resolution, and peak shape.

### Default settings:

Emission

•	Current:	mA
•	Protection Current:	3.5 mA
•	Ion Reference:	105 V
•	Cathode:	- 40.0 V
•	Focus:	-2.0 V
•	Field Axis:	-2.0 V
•	Extract:	-60 V

- 4. Optimize the ion source voltages:
  - a. Set "Field Axis" to -5 V.
  - b. Decrease "Field Axis" for useful resolution and peak shape.

## **Open High Sensitivity Ion Source**

This topic applies to the QMG220.

Proceed as follows to optimize the open high sensitivity ion source:

1. Select the filament and operate it with 2 mA emission current for approximately half an hour ("Protection Current" at 3.5 A). The message "Emission Error" appears repeatedly: start with reduced emission current and increase it slowly.

### Default settings:

•	Emission Current:	2 mA
•	Protection Current:	3.5 A
•	RF-Polarity:	pos
•	Ion Reference:	150 V
•	Cathode:	-75 V
•	Focus:	-5 V
•	Field Axis:	-7 V
•	Extract:	-50 V

- 3. Wait until the pressure reaches  $< 10^{-7}$  mbar and the residual gas spectrum remains stable.
- 4. Introduce a test gas, such as air, into the recipient for a pressure of 10-6 mbar. Otherwise, use the residual gas to perform the optimization procedure.
- 5. Repeatedly record spectra of the relevant peaks (e.g. 25...34 m/e). Observe intensity, resolution, and peak shape.
- 6. Optimize the ion source voltages:
  - a. Check which "RF-Polarity" ("pos" or "neg") results in the better peak shape and select this polarity.
  - b. Optimize "Cathode" for best sensitivity.
  - c. Adjust "Field Axis" for useful resolution and peak shape.

d. Optimize "Extract" and "Focus" alternately for maximum peak height.

## **Gastight High Sensitivity Ion Source**

This topic applies to the QMG220.

Proceed as follows to optimize the gastight high sensitivity ion source:

- Using air as test gas,
- Using argon and avoiding double ionization

### Using air if no specific test gas is available

1. Select the filament and operate it with 1 mA emission current for approximately half an hour ("Protection Current" at 3.5 A). The message "Emission Error" appears repeatedly: start with reduced emission current and increase it slowly.

Default settings for air as test gas:

•	Emission	1 mA
	Current:	
_	Drotoction	2 E A

• Protection 3.5 A Current:

RF-Polarity: posIon 150 V Reference:

Cathode: -60 V
Focus: -5 V
Field Axis: -7 V
Extract: -50 V

- 2. Repeatedly record spectra of the relevant peaks (e.g. 25...34 m/e). Observe intensity, resolution, and peak shape.
- 3. Optimize the ion source voltages:
  - a. Check which "RF-Polarity" ("pos" or "neg") results in the better peak shape and select this polarity.
  - b. Optimize "Cathode" for best sensitivity.
  - c. Adjust "Field Axis" for useful resolution and peak shape.

d. Optimize "Extract" and "Focus" alternately for maximum peak height.

The ion source is optimized.

### Using argon and avoiding double ionization

1. Select the filament and operate it with 1 mA emission current for approximately half an hour ("Protection Current" at 3.5 A). When the message "Emission Error" appears repeatedly start with reduced emission current and increase it slowly.

Default settings for argon as test gas:

•	Emission	1 mA
	Current:	

•	Protection	3.5 A
	Current:	

•	RF-Polarity:	pos
•	Ion	105 V
	Reference:	

•	Cathode:	-40 V
•	Focus:	-5 V
•	Field Axis:	-6 V
•	Extract:	-50 V

- 2. Repeatedly record spectra of the relevant peaks (e.g. 35...42 m/e). Observe intensity, resolution, and peak shape.
- 3. Optimize the ion source voltages:
  - a. Check which "RF-Polarity" ("pos" or "neg") results in the better peak shape and select this polarity.
  - b. Leave "Cathode" at -40 V to avoid double ionization.
  - c. Adjust "Field Axis" for useful resolution and peak shape.
  - d. Optimize "Extract" and "Focus" alternately for maximum peak height.

## **Tuning the Mass Scale**

## **Calibrating the Mass Scale**

#### **Basics**

Gas components are represented by integer mass numbers. Typically, the measuring apparatus causes small deviations between the nominal mass number and the actual position of the peak maximum. The correct position of the peak maxima is usually close to theoretical value, e.g. at 13.95 instead of 14.00. However, an exact measurement requires measuring the peak maximum. To achieve best accuracy in measurements, the exact position of the peak maxima has to be determined by calibrating the mass scale.

#### Procedure

QUADERA® uses two steps to calibrate the mass scale:

#### • Coarse tuning:

Two parameters are used to shift and to shrink or stretch the mass scale. This coarse tuning will be applied to all measurements.

#### • Fine tuning:

The fine tuning is based on the coarse tuning and compensates nonlinearity of the mass scale by manually entering corrected mass values. This fine tuning is applied to sample measurements and scan-stair measurements, and also to scan-analog measurements with the QMG700.

The Fine Tuning process is a manual process.

A **Mass Scale Adjust** template is provided that automates the determination of measured mass numbers. This template can be configured through the Recipe Editor; the decision to save or discard Mass Scale Tune Entries is still left to the user.

Mass Scale Adjust uses the following controls:

Update Mass List – Adds new masses from the Recipe into the Mass Adjust list. In order to update the Mass Adjust list, masses must first be entered into the Recipe as Measurement Tasks.

Remove Mass – Removes a selected Mass from the Mass Adjust list. This action has no effect on the Masses (Measurement Tasks) in the Recipe.

Apply to Mass Scale Table – Downloads the changes made in Mass Scale Adjust to the device Mass Scale Table. This action commits and saves the changes determined by QUADERA (and the device) into the device.

Reset Mass Scale Table – Resets all Actual Masses in the Mass Adjust list to their respective Reference Mass.

State column – The following states can occur when running Mass Scale Adjust:

 Ok: The calibration has been successfully performed; the exact mass numbers are shown in the column Actual Mass.

- Mass number too low: The entered mass number is too far to the left of the peak (i.e. too low in AMU).
- Mass number too high: The entered mass number is too far to the right of the peak (i.e. too high in AMU).
- Peak Intensity below threshold: Intensity lower than the level defined by the Threshold parameter.
- Peak Intensity too high: Intensity equal to or higher than full scale range.
- Peak width too narrow: The peak is too narrow to determine a maximum.
- Mass number too low; intensity tail too high: Intensity is too constant to determine a maximum.

Two scan analog measurements in various mass ranges are used for tuning of the mass scale. The <u>recipe parameters</u> are defined in the calibration project for the mass scale. Use the <u>recipe editor</u> to change the parameters. Normally, scanned masses range from one up to many masses.

#### NOTE

It is preferred that the two scans cover a mass range as wide as possible. One peak should appear at a very low mass number, another one at a very high mass number.

Scan recording begins when the calibration project is started. The currently set mass scale parameters are applied and displayed in the working area. Perform the tuning procedure during the course of the measurement: Modify the parameters to adjust the peak positions to the nominal mass numbers. You can observe the effect of modified parameters during the next cycle and iteratively tune the mass scale.

### **Coarse Tuning of the Mass Scale**

- 1. Feed a suitable calibration gas into the vacuum chamber. Use air if special calibration gases are not available.
- 2. Open the start page: In the View menu, click Show Start Page.
- 3. Click on the icon for the required device.
- 4. Only for QMG700: Reset the <u>fine tuning</u> data points before starting the coarse tuning procedure of the mass scale. Fine tuning is applied to scan analog measurements and will affect the coarse tuning.
- 5. Create a new calibration project: In the "Calibration and Tuning" list, double-click e.g. **Mass Scale Tuning (Coarse).qmt**. This way you create a new calibration project based on the selected template. You can modify it according to your needs.
- 6. The new measurement project window appears. The working area displays the calibration project.
  - <u>Edit the recipe</u> according to your needs (if necessary): Click the corresponding tab in the working area selection,
  - Display the measuring data: Click the corresponding tab in the working area selection.

#### NOTE:

You can start the measurement regardless whether the recipe editor or the working area has been selected.

- 7. Start the measurement: In the device status view, click on the "Start" icon. The connection to the device is automatically established. The device now receives the parameters for the current measurement task. You can adjust the chart layout while the measurement is running.
- 8. Adjust the actual peak positions to the nominal mass numbers: change the parameters in the section of the calibration project ("Mass Scale Tuning" editor) while the measurement is running. You can observe the effect of modified parameters during the next measurement task and iteratively tune the mass scale.
  - "Mass Scale Offset" shifts the mass scale,
  - "Mass Scale Slope" shrinks and stretches the mass scale.
- 8. Perform a <u>fine tuning</u> of the mass scale (if required). Otherwise, reset the fine tuning values to the default values.
  - 9. Stop the measurement: In the device status view, click on the "Stop" icon.
  - 10. Close and save the measurement project. In the **File** menu, click **Close**. You are requested if you want to save the measurement project. QUADERA® suggests an automatically generated file name that is based on date/time of the measurement and the used template.

- Yes: the "Save As" window used for saving measuring data opens up. Select a suitable name and path and then click **Save**. The measurement project will be saved and closed.
  - Please note: The file extension for measurement projects is \*.qmp
- No (recommended option): the measurement project will be closed without saving the data.
- Cancel: the action is cancelled. You will return to the measurement project without saving the data.

### NOTE:

The coarse tuning of the mass scale will be applied to all measurements.

## **Fine Tuning of the Mass Scale**

#### NOTE:

Perform the fine tuning of the mass scale exclusively within a coarse tuning procedure.

- 1. Feed a suitable calibration gas into the vacuum chamber. Use air if special calibration gases are not available.
- 2. Open the start page: In the **View** menu, click **Show Start Page**.
- 3. Click on the icon for the required device.
- 4. Create a new calibration project: In the "Calibration and Tuning" list, double-click e.g. Mass Scale Tuning (Fine).qmt. This way you create a new calibration project based on the selected template. You can modify it according to your needs.
- 5. The new measurement project window appears. The working area displays the calibration project.
  - Edit the recipe according to your needs (if necessary): Click the corresponding tab in the working area selection.
  - Display the measuring data: Click the corresponding tab in the working area selection.

#### NOTE:

You can start the measurement regardless whether the recipe editor or the working area has been selected.

- 6. Start the measurement: In the device status view, click on the "Start" icon. The connection to the device is automatically established. The device now receives the parameters for the current measurement task. You can adjust the chart layout while the measurement is running.
  - 7. Define the data points for the linear interpolation of the mass scale ("Mass Scale Tune Fine" editor):
  - a. Enter the nominal mass number in the "Nominal Mass" fields.
  - b. Enter the measured mass number in the "Actual Mass" fields (use the cursor to locate peak maximum).
    - 8. Adding and deleting data points:
    - Press ENTER when you have input the mass numbers. This way you add a row for a new data point.
    - Use the context menu of the "Mass Scale Tune Fine" editor to delete data points.
    - Delete all rows in the editor if there is no need for mass scale fine tuning: Click **Delete Mass Scale Tune Fine Entries**.

- 9. Stop the measurement: In the device status view, click on the "Stop" icon.
- 10. Close and save the measurement project. In the **File** menu, click **Close**. You are requested if you want to save the measurement project. QUADERA® suggests an automatically generated file name that is based on date/time of the measurement and the used template.
- Yes: the "Save As" window used for saving measuring data opens up. Select a suitable name and path and then click **Save**. The measurement project will be saved and closed.
  - Please note: The file extension for measurement projects is \*.qmp
- No (recommended option): the measurement project will be closed without saving the data.
- Cancel: the action is cancelled. You will return to the measurement project without saving the data.

#### NOTE:

The fine tuning of the mass scale will be applied to MID/MCD measurements and to scan-stair measurements, and also to scan-analog measurements with the QMG700.

NOTE: A Mass Scale Adjust template is provided that automates the determination of measured mass numbers. This template can be configured through the Recipe Editor; the decision to save or discard Mass Scale Tune Entries is still left to the user.

# **Parameters for Coarse Tuning**

Two parameters are used for coarse tuning, to shift and to shrink or stretch the mass scale. This way you can match the actual peaks with the nominal mass numbers.

The "Mass Scale Tune Coarse" editor in the calibration project displays the parameters for coarse tuning of the mass scale. Modified parameters are forwarded to the device and take effect in the next measurement cycle.

Image of "Mass Scale Tune Coarse" editor" (example)

Parameter	Range	Description
<ul> <li>Mass Scale Offset</li> </ul>	-0.12 < Offset < 0.12	Shift the mass scale to the left and right for negative and positive values, respectively.
<ul> <li>Mass Scale Slope</li> </ul>	0.985 < Slope < 1.015	Shrink and stretch the mass scale for values < 1.000 and > 1.000, respectively.



## **Parameters for Fine Tuning**

The fine tuning is based on the coarse tuning and compensates nonlinearity of the mass scale. You have to perform the fine tuning when the coarse tuning has been changed. Modified parameters are forwarded to the device and take effect in the next measurement cycle.

Data points on the mass scale have to be input for the fine tuning. These points are used for linear interpolation of mass numbers located in between. The "Mass Scale Tune Fine" editor lists the data points in a table. Use the context menu of this editor to delete data points.

Image of "Mass Scale Tune Fine" editor (example)

Pa	arameter	Range	Description
•	Nominal Mass	Integer number	Nominal mass number: Data point for the interpolation.
			<ul> <li>The listed values are sorted by increasing nominal mass number,</li> </ul>
			<ul> <li>Only one input is allowed per nominal mass.</li> </ul>
•	Actual Mass	+/- 0.5 amu around the nominal mass number	Measured mass number
•	Delete Mass Scale Tune Fine Entries	Button	Delete the data points input by the user in the "Mass Scale Tune Fine" editor.

### Context menu for the "Mass Scale Tune Fine" editor

In this context menu the following commands are available:

• **Delete selected rows:** Delete the selected rows, i.e. remove the data points.

Nominal Mass		Actual Mass
•	12	12.0
	18	18.1
	28	28.0
	32	32.0
	44	43.9

### Offset

#### Offset

#### **Basics**

The offset is caused by a drift of the measuring amplifier and can be compensated by a correction measurement. The measured intensity will be applied to future measurement projects by subtracting it from the results of the corresponding measurement tasks. You cannot switch on and off the offset values for saved data. If you wish to erase the stored values, there is a DELETE button in the Offset Calibration.qmt template in the Calibration and Tuning section.

#### Procedure

The measurement of the offset is performed by using the Offset Calibration.qmt template in the Calibration and Tuning section. Instead, the offset of the electronic circuit of the measuring amplifier is determined for each measuring range at a user-defined mass number. The values are automatically stored in the device and will remain after the power has been cut.

## **Determining the Offset**

#### NOTE:

Determine the offset for the electrometer preamplifier and detector, which you intend to use in the subsequent measurement:

- QMG220: one electrometer preamplifier is used with both detectors (if installed), i.e. there is only one set of offset values,
- QMG700: individual electrometer preamplifiers are used with both detectors (if installed), i.e. there are two different sets of offset values.
- 1. Open the start page: In the **View** menu, click **Show Start Page**.
- 2. Click on the icon for the required device.
- 3. Create a new calibration project: In the "Calibration and Tuning" list, double-click e.g. **Offset Calibration.qmt**. This way you create a new calibration project based on the selected template. You can modify it according to your needs.
- 4. The new measurement project window appears. The working area displays the calibration project.
- 5. Only QMG700:

Select the detector corresponding to the measuring amplifier ("Electrometer Preamplifier") whose offset is to be determined:

- Faraday,
- SEM.
- 6. Edit the mass ("Offset Mass") for the offset measurement.
- 7. Start the measurement: In the device status view, click on the "Start" icon. The connection to the device is automatically established. The device now receives the parameters for the current measurement task. The measurement runs automatically and should take about 10...15 s.
- 8. QUADERA® calculates the necessary offset values. The values are automatically stored for the individual measuring ranges of the amplifier and applied to future measurement projects.
  - 9. Close and save the measurement project. In the **File** menu, click **Close**. You are requested if you want to save the measurement project. QUADERA® suggests an automatically generated file name that is based on date/time of the measurement and the used template.
  - Yes: the "Save As" window used for saving measuring data opens up. Select a suitable name and path and then click Save. The measurement project will be saved and closed.
    - Please note: The file extension for measurement projects is \*.qmp
  - No (recommended option): the measurement project will be closed without saving the data.
  - Cancel: the action is cancelled. You will return to the measurement project without saving the data.

## **Offset Parameters**

The calibration project displays the parameters required to determine the offset. Modified parameters are forwarded to the device and take effect in the next measurement task.

### Offset parameters QMG220

Pa	arameter	Range	Description
•	E-05  E-12	(not editable)	Offset value for the corresponding measuring range of the detector.
			The device automatically determines the values listed in the corresponding table.
			See also <u>recipe parameter</u> "Amplifier Range".
•	Offset Mass	0 <= value <= MaxRange	Mass for the offset measurement.
•	Delete Offset Entries	Button	Deletes the offset values for the detector.

# Offset parameters QMG700

Pa	arameter	Range	Description
•	E-05  E-12	(not editable)	Offset value for the corresponding measuring range of the selected detector.
			The device automatically determines the values listed in the corresponding table.
			See also <u>recipe parameter</u> "Amplifier Range".
•	Electrometer Preamplifier	Dropdown list	Detector type for the offset determination.
			• Faraday,
			• SEM
•	Offset Mass	0 <= value <= MaxRange	Mass for the offset measurement.
•	Delete Offset Entries	Button	Deletes the offset values for the detector that is selected in

"Electrometer Preamplifier".

# **Tuning the RF Generator**

# **Tuning the RF Generator**

### **Basics**

The high frequency voltage of the RF generator (QMH, or RF22x for QMG220, see <u>device settings</u>) is applied to the rod pairs of the QMG to separate ions. The output resonant circuit of the generator has to be matched to the QMG rod system in the following cases:

- when commissioning the device,
- problems appear when masses near the upper mass scale limit are measured.

#### **Procedure**

Tuning the RF generator requires to turn the tuning screw. The calibration project in QUADERA® is used to display and check the tuning voltage.

#### NOTE:

Use the device specific instructions (OEM manual) when tuning the RF generator.

- Tuning the RF generator for the QMG220,
- Tuning the RF generator for the QMG700.

# Minimizing the Tuning Voltage (QMG220)

This topic applies to the QMG220.

#### NOTE:

Use the device specific instructions (OEM manual) when tuning the RF generator.

- 1. Open the start page: In the View menu, click Show Start Page.
- 2. Click on the icon for the required device.
- 3. Create a new calibration project: In the "Calibration and Tuning" list, double-click **RF Tuning.qmt** or **Tune Data.qmt**. This way you create a new calibration project based on the selected template.

# NOTE: The mass settings of Tune Data.qmt should be adjusted before tuning the RF generator.

- 1. The new measurement project window appears. The working area displays the calibration project. Note:
  - No recipe is assigned to this calibration project (RF Tuning.qmt). Thus, no user specific adaptation is available.
  - An actual measurement is not performed, i.e. you can not start and stop the measurement.
  - 5. Proceed as follows to tune the output resonant circuit of the generator:
  - Observe the signal bar in the working area. It displays the actual generator tuning voltage. The two drag indicators show the maximum and minimum achieved voltage.
  - Use the **Reset Arrows** command of the context menu "Chart" to reset the two drag indicators.
    - Not available in Tune Data.gmt.
  - Adjust the tuning screw of the generator to minimize the tuning voltage.
     Refer to the OEM manual. The tuning voltage should not exceed half of the maximum signal.

#### NOTE:

Do not damage the tuning screw of the generator. Never tighten or remove the tuning screw.

- 6. Close and save the measurement project. In the **File** menu, click **Close**. You are requested if you want to save the measurement project. QUADERA® suggests an automatically generated file name that is based on date/time of the measurement and the used template.
- Yes: the "Save As" window used for saving measuring data opens up. Select a suitable name and path and then click Save. The measurement project will be saved and closed.

Please note: The file extension for measurement projects is \*.qmp

- No (recommended option): the measurement project will be closed without saving the data.
- Cancel: the action is cancelled. You will return to the measurement project without saving the data.

### Extended context menu "Chart"

In the calibration project "RF Tuning" the context menu "Chart" provides an additional command:

• Reset Arrows Reset the drag indicators that show the maximum and minimum achieved tuning

voltago

# **Minimizing the Tuning Voltage (QMG700)**

This topic applies to the QMG700.

#### NOTE:

Use the device specific instructions (OEM manual) when tuning the RF generator.

- 1. Open the start page: In the View menu, click Show Start Page.
  - 2. Click on the icon for the required device.
- 3. Create a new calibration project: In the "Calibration and Tuning" list, double-click **RF Tuning.qmt** or **Tune Data.qmt**. This way you create a new calibration project based on the selected template.
- 4. The new measurement project window appears. The working area displays the calibration project. Note:
  - No recipe is assigned to this calibration project. Thus, no user specific adaptation is available.
  - An actual measurement is not performed, i.e. you can not start and stop the measurement.
  - 5. The QMH is set to the maximum mass number in **RF Tuning.qmt**. Tune the output resonant circuit as described in the instructions of the RF generator.

NOTE: The mass settings of Tune Data.qmt should be adjusted before tuning the RF generator.

### NOTE:

Do not damage the tuning screw of the generator. Never tighten or remove the tuning screw.

- 6. Close and save the measurement project. In the **File** menu, click **Close**. You are requested if you want to save the measurement project. QUADERA® suggests an automatically generated file name that is based on date/time of the measurement and the used template.
  - Yes: the "Save As" window used for saving measuring data opens up. Select a suitable name and path and then click **Save**. The measurement project will be saved and closed.
    - Please note: The file extension for measurement projects is \*.qmp
  - No (recommended option): the measurement project will be closed without saving the data.
  - Cancel: the action is cancelled. You will return to the measurement project without saving the data.

# **Background Determination**

# **Background Determination**

### **Basics**

The mass spectrometer background is caused by residual gases. These gases are present in every analysis chamber and do not originate from the measuring sample. The background is mainly constant if the measuring apparatus is well conditioned. However, measurement results may be distorted if the background is not considered properly. The background determination identifies the existing residual gases. The detected ion currents are subtracted from subsequent measurement projects. The result will show the true composition of the measuring gas.

#### Procedure

Residual gases are measured either with the gas inlet closed or by using a zero gas, i.e. a pure gas that is fed into the analysis chamber to reach the same pressure as expected for future measurements. Using a zero gas takes account of adsorption and desorption effects better than pumping down the chamber to final vacuum.

An MID measurement is used to determine the background. The <u>recipe parameters</u> are defined in the corresponding calibration project. Use the <u>recipe editor</u> to change the parameters. You can determine the mass spectrometer background for **each detector type separately** and store the results in the Background Library. The stored values will be used in future MID and MCD measurement projects where they are subtracted from the measured signals.

### NOTE:

Always pump down the chamber to final vacuum before performing the background determination, or let in a suitable zero gas. Otherwise, serious measurement errors may result.

# Measuring the Background

### NOTE:

Before starting the measurement, check the correct calibration of the mass spectrometer components. If a calibration is necessary, perform the following preparatory measurements:

- Calibrate the mass scale,
- Determine the offset.
- 1. Feed a suitable zero gas into the vacuum chamber, or pump the chamber down to final vacuum.
- 2. Open the start page: In the View menu, click Show Start Page.
- 3. Click on the icon for the required device.
- 4. Create a new calibration project: In the "Templates" list, double-click e.g. **Background Determination.qmt**. This way you create a new calibration project based on the selected template. You can modify it according to your needs.
- 5. The new measurement project window appears. The working area displays the calibration project.
  - <u>Edit the recipe</u> according to your needs (if necessary): Click the corresponding tab in the working area selection.
     The measurement tasks must not contain mass numbers where peaks of the zero gas appear.
  - Display the measuring data: Click the corresponding tab in the working area selection.

### NOTE:

You can start the measurement regardless whether the recipe editor or the working area has been selected.

- 6. Start the measurement: In the device status view, click on the "Start" icon. The connection to the device is automatically established. The device now receives the parameters for the current measurement task. The measurement is running automatically.
- 7. Check the measured values, e.g. display the measuring data in a table.
- 8. Click **Apply to Background Library** to forward the background measurement to the Background Library. Note:
  - New background measurements (mass numbers) are added to the Background Library,
  - Current measuring values replace existing data sets in the Background Library.
- 9. Close and save the measurement project. In the **File** menu, click **Close**. You are requested if you want to save the measurement project. QUADERA® suggests an

automatically generated file name that is based on date/time of the measurement and the used template.

- Yes: the "Save As" window used for saving measuring data opens up. Select a suitable name and path and then click **Save**. The measurement project will be saved and closed.
  - Please note: The file extension for measurement projects is \*.qmp
- No (recommended option): the measurement project will be closed without saving the data.
- Cancel: the action is cancelled. You will return to the measurement project without saving the data.

### NOTE:

The data sets in the Background Library will be subtracted in MID and MCD measurements. If you wish to skip this subtraction then reset the data sets in the Background Library ("Delete Background Library" button). Background Subtraction can also be disabled, without resetting the Background Library, from the context menu when running a Measurement Project.

# **Background Library**

The Background Library in the section of the calibration project displays the parameters required to determine the background. Changed parameters take effect in the next measurement task.

The Background Library contains the corresponding background data for all measured mass numbers in tabular form. You can use various zero gases and perform consecutive background determinations. The results can be combined in the Background Library (function "Apply to Background Library"). Note that an individual Background Library is created for each installed detector.

Image of background library (example)

Parameter	Range	Description
• Detector	Dropdown list	The Background Library is displayed for the selected detector type:
		<ul> <li>Faraday: the table for the Faraday detector is displayed.</li> </ul>
		<ul> <li>SEM: the table for the SEM detector is displayed.</li> </ul>
		<ul> <li>IonCounter (only QMG700): the table for the ion counter is displayed.</li> </ul>
• Mass	Mass number (not editable)	Mass number for which the background has been determined: applied from the related MID recipe ("Mass" parameter).
<ul> <li>Intensity</li> </ul>	Measured value	Background intensity at the related mass number: corresponds to the currently measured value for this mass number.
<ul> <li>Apply to Background Library</li> </ul>	Button	Apply the result of the current background determination to the Background Library for the detector that is selected in the recipe.
		NOTE:
		<ul> <li>New background measurements are added to the Background Library,</li> </ul>
		<ul> <li>Current measuring values replace existing data sets in the Background Library.</li> </ul>

Delete Background Library Button

Delete all data sets of the Background Library, for all detectors.

### NOTE:

"Delete Background Library" deletes the data sets of the Background Library irretrievably. In this case, a new background determination is required for new data sets.

# QUADERA HTML Help

	Mass 4	Intensity
	14	2,2100E-11 A
•	16	1,5300E-11 A
18		4,8900E-10 A
	28	3,8700E-10 A
32		8,4600E-11 A
	40	5,9300E-12 A
	44	5,9300E-12 A

# **Gas Specific Calibration**

### **Gas Specific Calibration**

### NOTE:

Perform the following preparatory measurements before the gas specific calibration:

- Calibrate the mass scale,
- Determine the offset,
- Determine the background.

#### **Basics**

An MCD measurement project uses a matrix of calibration factors (analysis matrix) to convert ion currents into gas concentrations. The calibration factors are not universally valid. They have to be quantified by a separate calibration measurement using known gases (calibration gases). Calibration gases are selected according to the components in the measurement project whose concentrations are to be measured.

### NOTE:

Gas mixtures that contain components with overlapping masses are not suited for use as calibration gas. The same mass number must not be assigned to several components.

### Procedure

One MID measurement project is created per calibration gas. The <u>recipe parameters</u> include the mass numbers of the calibration gas components and can be modified in the <u>recipe editor</u>. The "GSC Matrix" editor specifies the concentration of each calibration gas component and its contribution on the related mass number. The gas specific calibration factors are required for the actual MCD measurement project. They are determined in the calibration project (<u>GSC Result View</u>) and saved in the <u>MCD Calibration Factor Library</u>.

# **Determining the GSC Factors**

#### NOTE:

Before starting the measurement, check the correct calibration of the mass spectrometer components. If calibration is necessary, perform the following preparatory measurements:

- Calibrate the mass scale,
- Determine the offset.
- Determine the background.

#### NOTE:

Gas mixtures that contain components with overlapping masses are not suited for use as calibration gas. The same mass number must not be assigned to several components.

- 1. Feed a suitable calibration gas into the vacuum chamber.
- 2. Open the start page: In the View menu, click Show Start Page.
- 3. Click on the icon for the required device.
- 4. Create a new calibration project: In the "Templates" list, double-click e.g. **Gas Specific Calibration.qmt**. This way you create a new calibration project based on the selected template. You can modify it according to your needs.
- 5. The new measurement project window appears. The working area displays the calibration project.
  - Edit the recipe according to your needs (if necessary): Click the corresponding tab in the working area selection.
  - Display the measuring data: Click the corresponding tab in the working area selection.
- 6. Input the parameters which define the calibration gas in the "GSC Matrix" editor.
  - Use the commands of the related context menu to edit the measurement tasks and masses.
  - Note: Use an identical name for the gas component in an MCD project.
     Otherwise, QUADERA® cannot refer to this component. As an example,
     QUADERA® does not equate "O2" and "Oxygen".

### NOTE:

You can start the measurement regardless whether the recipe editor or the working area has been selected.

- 7. Start the measurement: In the device status view, click on the "Start" icon. The connection to the device is automatically established. The device now receives the parameters for the current measurement task. The measurement is running automatically.
- 8. In the <u>GSC Result View</u>, check the measured values and the calculated calibration factors.

- 9. Click **Apply to MCD Calibration Factor Library** to save the calibration factors in the <u>MCD calibration factor library</u>. Note:
  - New calibration factors are added to the MCD Calibration Factor Library,
  - Current values replace existing data sets in the MCD Calibration Factor Library.
- 10. When required for future applications: save the calibration project as template (menu File > Save as Template...).
- 11. Close and save the measurement project. In the **File** menu, click **Close**. You are requested if you want to save the measurement project. QUADERA® suggests an automatically generated file name that is based on date/time of the measurement and the used template.
  - Yes: the "Save As" window used for saving measuring data opens up. Select a suitable name and path and then click **Save**. The measurement project will be saved and closed.
    - Please note: The file extension for measurement projects is \*.qmp
  - No (recommended option): the measurement project will be closed without saving the data.
  - Cancel: the action is cancelled. You will return to the measurement project without saving the data.

# **GSC Matrix Editor**

The parameters that define the calibration gas are displayed in the "GSC Matrix" editor of the calibration project. Each calibration gas component is defined by its name, concentration, and the measurement task(s). Use the "Add MCD Task" tool to add a new component (measurement task).

Image of "GSC Matrix" editor (example)

Parameter	Range	Description
<ul> <li>Component</li> </ul>	Letters and digits	Name of the calibration gas component.
		Note: In an MCD project, use an identical name for the gas component. Otherwise, QUADERA® cannot refer to this component. As an example, QUADERA® does not equate "O2" and "Oxygen".
Concentration	Number > 0	Concentration of the calibration gas component.
• Mass	(not editable)	The gas specific calibration factors are determined for these measurement tasks: accepted from the MID recipe ("Task Name" parameter).
• Mass #	Checkbox	Defines whether a calibration factor for the component is determined in the corresponding measurement task, or not.
		Note:
		<ul> <li>Only one calibration factor can be calculated per measurement task.</li> </ul>
		<ul> <li>Several calibration factors per component can be determined at the same time.</li> </ul>
		<ul> <li>A red colored cell indicates the internal standard. Use the context menu of the "GSC Matrix" editor to set the internal standard.</li> </ul>

Context menu of the "GSC Matrix" editor

In this context menu the following commands are available:

- **Delete selected Component**: delete the marked measurement task (table row) from the "GSC Matrix" editor.
- **Delete selected Mass**: delete the marked mass (table column) from the "GSC Matrix" editor.
- Set as internal standard: set the internal standard for the calibration factors.

Proceed as follows to set the internal standard for the calibration factors:

- 1. Open the context menu in the table element related to the mass/component pair you want to set as internal standard.
- 2. Click **Set as internal standard**. The table element for the internal standard appears with a red background color.

# QUADERA HTML Help

Mass				ass				
	Component	Concentration	Mass 14	Mass 28	Mass 29	Mass 32	Mass 40	Mass 44
١	Ar	0.93%					~	
	CO2	300ppm						>
	N2	78.14%	~	<	>			
	02	20.9%				>		

### **GSC Result View**

The parameters required to determine the calibration factors are displayed in the "GSC Result View" of the calibration project.

The "GSC Result View" displays the calibration factors in a tabular form. They are calculated for all measurement tasks of the MID recipe, using the corresponding measured data. In the course of time you can extend and complete the MCD Calibration Factor Library (function "Apply to MCD Calibration Factor Library") by using various calibration gases to determine the calibration factors.

Image of "GSC Result View" (example)

Parameter		Range	Description
•	Component	(not editable)	Name of the calibration gas component: applied from the "GSC Matrix" editor ("Component" parameter).
•	Mass	(not editable)	Measurement tasks for which the gas specific calibration factors are determined: applied from the related MID recipe ("Task Name" parameter).
•	Intensity	(not editable)	Intensity at the related mass number: corresponds to the currently measured value for this mass number.
•	Factor	(not editable)	The calibration factor is automatically calculated from the measured intensity and the specified concentration.
•	Apply to MCD Calibration Factor Library	Button	Apply the current gas specific calibration factors to the MCD Calibration Factor Library.
			NOTE:
			<ul> <li>New calibration factors are added to the MCD Calibration Factor Library,</li> </ul>
			<ul> <li>Current values replace existing data sets in the MCD Calibration Factor Library.</li> </ul>

# QUADERA HTML Help

	Component	Mass	Intensity	Factor	
	02	Mass 32	8,124E-06	3,111E00	
•	N2	Mass 28	9,764E-06	1,000E00	
	Ar	Mass 40	1,630E-06	1,403E01	
	C02	Mass 44	6,150E-08	1,641E01	

# **MCD Calibration Factor Library**

Measuring the concentration of the components of a gas mixture requires that the corresponding calibration factors are known. These are stored in the MCD Calibration Factor Library, in tabular form. Each calibration factor is defined in the related calibration project by the mass number and the name of the corresponding component.

The calibration factors are quantified relatively. This requires to set one calibration factor as the internal standard. Normally, the calibration factor for  $N_2$  (m/e = 28) is used and set to 1 (standard setting). The other calibration factors relate to the standard. This approach allows you to create a consistent MCD Calibration Factor Library. Use the context menu of the "GSC Matrix" editor to set the internal standard.

Image of MCD Calibration Factor Library (example)

### **Extending the MCD Calibration Factor Library**

Proceed as follows to extend the MCD calibration factor library:

- 1. Perform a new gas specific calibration (calibration project).
- Apply the new calibration factors to the MCD Calibration Factor Library: In the section of the calibration project, click Apply to MCD Calibration Factor Library.

### **Deleting the MCD Calibration Factor Library**

 Click Delete MCD Calibration Factor Library to remove all data sets from the MCD calibration factor library.

#### NOTE:

"Delete MCD Calibration Factor Library" deletes the data sets of the MCD Calibration Factor Library irretrievably. In this case, a new gas specific calibration is required for new data sets.

# QUADERA HTML Help

	MCD Calibration Factor Library						
Mass 🛆	14,00	16,00	18,00	28,00	32,00	40,00	44,00
Factor H20	0,00	0,01	1,00	0,00	0,00	0,00	0,00
Factor Ar	0,00	0,00	0,00	0,00	0,00	1,00	0,00
Factor 02	0,00	0,10	0,00	0,00	0,87	0,00	0,00
Factor N2	0,10	0,00	0,00	1,00	0,00	0,00	0,00
Factor CO2	0,00	0,00	0,00	0,20	0,00	0,00	1,50

# **Enabling Partial Pressure**

# **Determining the Sensitivity**

The Device Sensitivity must be determined for the device to display Partial Pressure.

To determine the Sensitivity, run the Sensitivity Determination measurement project. Enter the Calibration Factors for each mass, enter the Total Pressure (if no gauge is attached) and run the measurement project.

The Device Sensitivity can then be saved to the software device.

# **Required Process to Enable Partial Pressure**

To use Partial Pressure, the following must be done:

- An <u>Offset Calibration</u> must have been executed at some point. QUADERA will check to see if this has been done.
- A SEM Amplification Calibration must have been executed at some point. This
  determines the gain of the SEM.
- Calibration Factors must be set up using the <u>Sensitivity Determination</u> measurement project.
- The Sensitivity must be determined for the device using the <u>Sensitivity</u> <u>Determination</u> measurement project. A default Sensitivity is available but is not as accurate as a Sensitivity determined by QUADERA for the specific device.
- The Partial Pressure units must be selected (default is mbar).

# Measurements using QUADERA

# **Measurement Projects and Measurement Project Templates**

In QUADERA®, data are stored as measurement project templates and as measurement projects. Each measurement project template or measurement project is used for a specific measurement task.

# Measurement project templates

Measurement project templates allow you to access frequently performed measurement tasks easily. Measurement project templates are created by INFICON or experienced users in order to keep the effort required for configuring typical measurement tasks at a minimum. Typical measurement project templates are installed together with QUADERA®. You can find these in the <u>Start page</u>.

In addition, QUADERA® provides basic templates for each measurement project, such as Scan, MID, MCD etc. These templates normally include just one measurement task and are intended to create user specific measurement project templates as starting points for future measurement projects.

### Measurement projects

A measurement project contains the measuring data as well as an image of the device required for displaying the measuring data correctly.

	Measurement project template	Measurement project
File extension	*.QMT	*.QMP
Recipe definition	Yes	Yes
Configured sections	Yes, several	Yes, several
Device settings	Reference to the device type	Complete image of the device
Measuring data	No	Yes

Comparison: Measurement project template vs. measurement project

# **Scan Measurement Projects**

In a scan-analog measurement, the ion current is measured as a function of m/e. This quickly allows you to make a qualitative statement such as "The gas consists of ..., ..., ..., of which ... represents the majority. The fraction of ... is very small or cannot be measured".

However, it is rather cumbersome to deduce the quantitative composition of the gas in % or ppm. Information about changes in the gas composition with time is hard to deduce from a sequence of several scans, and measurements over long periods of time also result in extremely large amounts of data.

In scan-analog measurement projects you can also add analog input tasks (e.g. via quadrupole controller QC, "EXT IN").

Scan-analog also allows for capturing and comparing a reference scan if using a reference-based measurement project.

A separate measurement project - Bargraph Cycles - can be used to plot analog scans against time.

QUADERA® also provides a scan-analog measurement project template that displays a 3D graph of analog scans. 3D consumes system resources and should be used for only short periods of time, if possible.

### NOTE:

A precise measurement requires the correct <u>calibration</u> of the components of the mass spectrometer.

See <u>Example for the course of a scan measurement project</u> (measure\_example\_scan).

### NOTE:

For a written documentation of your measurement projects you can <u>capture</u> <u>screens</u> of the QUADERA® user interface. Reports can also be printed from a selection on the context menu.

# **MID Measurement Projects**

In an MID measurement (Multiple Ion Detection) you specify distinct m/e values for which the ion current is to be measured. Only the specified mass numbers are scanned in this case. Each of these mass numbers is represented by a separate measurement task for which all parameters can be set.

Changes in the gas composition with time can be recorded and displayed easily. An additional analysis of the measuring data allows you to convert the results into concentrations given in %, ppm, etc (MCD measurement).

MID Measurement data can be displayed in amps or partial pressure. To display in partial pressure, one must first run the offset calibration measurement, calibrate the SEM Amplification, then determine the device sensitivity and lastly set the partial pressure units.

- The Sensitivity of the instrument is the ratio of the ion current measured for a given mass to the partial pressure of a gas.
- Only one Sensitivity parameter exists in QUADERA. It is used to calculate Partial Pressures for measurements using the Faraday or SEM detector.
- Partial Pressure also uses a Calibration Factor, which is the ratio of the total ion current (at all masses) produced from a given partial pressure of that substance, to the total ion current produced from nitrogen at the same partial pressure. The Calibration Factor(s) depends strongly on the energy of the ionizing electrons. If the correct values of the Calibration Factors are not known for the exact conditions of the particular analyzer being used, they can be approximated using published relative ion gauge sensitivities for various gases.
- If the SEM voltage is changed after SEM Amplification and Sensitivity have been determined then Partial Pressure calculations will be less accurate. If changing the SEM voltage, it is best to calibrate the SEM Amplification and determine the Sensitivity again before using Partial Pressure.

NOTE: Setting or changing the partial pressure units requires one full scan through the MID measurement tasks to correctly update the chart.

### NOTE:

A precise measurement requires the correct <u>calibration</u> of the components of the mass spectrometer.

See <u>Example for the course of an MID measurement project</u> (measure\_example\_sample).

### NOTE:

For a written documentation of your measurement projects you can <u>capture</u> <u>screens</u> of the QUADERA® user interface. Reports can also be printed from a selection on the context menu.

# **MCD Measurement Projects**

The MCD measurement (Multiple Concentration Determination) is based on an MID measurement project and includes additional evaluation to measure concentrations. A matrix of calibration factors (analysis matrix) is used to convert the measured ion currents into concentrations of the individual gas components. The calibration factors are not universally valid. They must be quantified by a separate measurement using calibration gases, i.e. one or more GSC measurements. The actual MCD measurement and the calibration are closely connected.

### NOTE:

A precise measurement requires the correct <u>calibration</u> of the mass spectrometer components.

- 1. Before starting the measurement, check the correct calibration of the components of the mass spectrometer. If calibration is necessary, perform the following preparatory measurements:
  - Calibrate the mass scale,
  - Measure the offset,
  - Determine the background of the mass spectrometer,
  - Quantify the gas specific calibration factors.
- 2. Open the start page: In the View menu, click Show Start Page.
- 3. Click on the icon for the required device.
- 4. Create a new MCD measurement project: In the "Templates" list, double-click the desired measurement project template. This way you create a new measurement project based on the selected template.
  - 5. The new measurement project window appears. The working area displays the MCD project.
  - Edit the MCD recipe if necessary: click the corresponding tab in the working area selection,
  - Display the measuring data: click the corresponding tab in the working area selection.

### NOTE:

You can start the measurement regardless whether the recipe editor or the working area has been selected.

- 6. Start the measurement: In the device status view, click on the "Start" icon. The connection to the device is automatically established. The device now receives the parameters for the current measurement task. You can adjust the chart layout while the measurement is running.
  - 7. Stop the measurement: In the device status view, click on the "Stop" icon.
  - 8. Close and save the measurement project. In the **File** menu, click **Close**. You are requested if you want to save the measurement project. QUADERA®

suggests an automatically generated file name that is based on date/time of the measurement and the used template.

- Yes: the "Save As" window used for saving measuring data opens up. Select a suitable name and path and then click **Save**. The measurement project will be saved and closed.
  - Please note: The file extension for measurement projects is \*.qmp
- No: the measurement project will be closed without saving the data.
- Cancel: the action is cancelled. You will return to the measurement project without saving the data.

### NOTE:

For a written documentation of your measurement projects you can <u>capture</u> <u>screens</u> of the QUADERA® user interface. Reports can also be printed from a selection on the context menu.

### **Total Pressure Measurement**

This chapter is valid for the QMG220 only.

QUADERA® supports total pressure measurements in the vacuum system (hardware supported only for QMG220). This requires that an appropriate pressure gauge is connected to the QMG and the <u>device settings are adjusted</u> accordingly. The total pressure measurement is available for:

- Scan measurement projects,
- MID measurement projects,
- MCD measurement projects.

Use the <u>recipe editor</u> to add the measurement task "Total Pressure" to the measurement project. The measured data (total pressure in the vacuum system) are displayed and saved. Besides, the course of a measurement corresponds to the selected measurement project.

### Adding the measurement task "Total Pressure" to a recipe

Apply the "Add Total Pressure Task" or "Add Total Pressure Task to Chart" tools to the recipe editor. Edit the <u>recipe parameters</u> if necessary.

### **Further notes**

Pay attention to the following items when measuring the total pressure:

- The pressure gauge is not permanently switched on because the plasma in the gauge influences the gas composition in the recipient. Exception: monitoring the QMG.
- Note that igniting the pressure gauge and displaying the correct pressure will take some time (refer to the operating instructions for the pressure gauge).

### NOTE:

For a written documentation of your measurement projects you can <u>capture</u> <u>screens</u> of the QUADERA® user interface. Reports can also be printed from a selection on the context menu.

# **Creating Measurement Project Templates**

Proceed as follows to create a new measurement project template:

- 1. Use e.g. the <u>start page</u> to open an existing measurement project template, or an existing measurement project.
- 2. Use the <u>recipe editor</u> to modify the recipe parameters according to your needs.
- 3. Use the <u>toolbox</u> to change the working area according to your needs.
- 4. In the **File** menu, click **Save As Template...**. Select the path for the measurement project template, and input the file name.

### Note:

- By default, the path set in the <u>options</u> is used for new measurement project template,
- The file extension \*.qmt is used for measurement project templates.

# **Recipes**

# Recipes

A recipe contains a sequence of measurement tasks. Use the <u>recipe editor</u> to change the recipe parameters.

The following recipe types are available:

• Scan recipes: parameters for scan-analog measurement project

In a scan-analog measurement, the ion current is measured as a function of m/e. This quickly allows you to make a qualitative statement such as "The gas consists of ..., ..., of which ... represents the majority. The fraction of ... is very small or cannot be measured".

However, it is rather cumbersome to deduce the quantitative composition of the gas in % or ppm. Information about changes in the gas composition with time is hard to deduce from a sequence of several scans, and measurements over long periods of time also result in extremely large amounts of data.

In scan-analog measurement projects you can also add total pressure measurement tasks (for the QMG220, if a pressure gauge is installed) and analog input tasks (AI).

• <u>MID recipes</u>: parameters for *MID/MCD measurement project* 

In an MID measurement (Multiple Ion Detection) you specify distinct m/e values for which the ion current is to be measured. Only the specified mass numbers are scanned in this case. Each of these mass numbers is represented by a separate measurement task for which all parameters can be set. Changes in the gas composition with time can be recorded and displayed easily. An additional analysis of the measuring data allows you to convert the results into concentrations given in %, ppm, etc. (MCD measurement). In MID measurement projects you can also add total pressure measurement tasks (for the QMG220, if a pressure gauge is installed) and analog input tasks (AI).

MCD recipes: additional parameters for MCD measurement project

The MCD measurement (Multiple Concentration Determination) is based on a MID measurement project and includes additional evaluation to measure concentrations. A matrix of calibration factors (analysis matrix) is used to convert the measured ion currents into the concentrations of the individual gas components. The calibration factors are not universally valid. They have to be quantified by a separate measurement using calibration gases. In MCD measurement projects you can also add total pressure measurement tasks (for the QMG220, if a pressure gauge is installed) and analog input tasks (AI).

# NOTE:

New or modified parameters for the measurement tasks are accepted by the device only after the measurement has been restarted.

# **Recipe Editor**

In the working area selection, click the corresponding tab. The recipe parameters for the active recipe are displayed in the section in tabular form (recipe editor). The columns represent the measurement tasks and the rows represent the recipe parameters.

### **Editing parameters**

Proceed as follows to edit a parameter:

- 1. Click the required cell.
- 2. Depending on the parameter type:
  - Enter the required parameter via the keyboard, or
  - Use the spin buttons to modify the parameter, or
  - Select the required parameter in the respective dropdown list.
  - 3. After a parameter has been input, an automatic check is normally performed to ensure that the parameter lies within the permitted range. This prevents bad data input, and facilitates correct input.
  - 4. The parameter is accepted automatically as soon as you leave the cell.

### Add measurement task

Proceed as follows to add a new measurement task to the recipe:

- 1. Use the tool that is applicable to the measurement project:
  - "Add Scan Task" for scan measurement projects.
  - "Add Peak Task" for scan measurement projects.
  - "Add MID Task" for MID and MCD measurement projects.
  - "Add MCD Task" for MCD measurement projects.
  - "Add Total Pressure Task" for Scan, MID and MCD measurement projects,
  - "Add Analog Input Task" for Scan, MID and MCD measurement projects.

# Change sequence of measurement tasks

Proceed as follows to change the sequence of measurement tasks in a recipe:

- 1. Select the column that corresponds to the measurement task.
- 2. Drag&Drop the measurement task to the required position. A red arrow indicates the insert position.

### Delete measurement task

Proceed as follows to delete a measurement task from the recipe:

- 1. Select the entire column that corresponds to the measurement task.
- On the keyboard, click the **Del** key (delete), or use the context menu. When the measurement task contains data a requester appears and queries you to approve deleting.

### Context menu of the recipe editor

This context menu contains the following functions

- Copy Parameter To All: applies the selected parameter to all measurement tasks.
- **Delete selected Task**: deletes the selected measurement task.

### NOTE:

New or modified parameters for the measurement tasks are accepted by the device only after the measurement has been restarted.

# **Recipe Parameters: Scan**

### NOTE:

New or modified parameters for the measurement tasks are accepted by the device only after the measurement has been restarted.

The following recipe parameters are available:

Task Name

First Mass

Width

**Speed** 

**Dwell** 

Mass Mode

**Detector Type** 

**Al Channel** 

Gain (only QMG700)

**SEM Voltage** 

CP-Level (only QMG700)

**Autorange Mode** 

**Detector Range** 

Range Limit

Analog Signal Filter (only QMG700)

Resolution

Pause Calibrate

**AO Channel** 

AO Mode (only QMG220)

AO Range (only QMG220)

Trip Type

Level A

DO# A

Level B

<u>DO# B</u>

**State** 

Parameter Range Description

	Task Name	Letters and	Name of the measurement task.
	raskriams	digits	Note that for analog input scan measurement tasks the <u>trip function</u> and the related parameters are available.
•	First Mass	Number > 0	Start mass for the measurement.
			Enter the required value or use the spin buttons.
•	Width	Any number	Mass range to be scanned (starting with the start mass). Reverse scans, i.e. from right to left, are performed for negative values.
			Enter the required value or use the spin buttons.
•	Speed	Dropdown list	Measuring time per mass for scan measurements (mass scan)
•	Dwell	Dropdown list	Dwell time for the measurement of the analog input of the QC (only relevant for detector type EXT_IN_# in analog input measurement tasks).
•	MassMode	Dropdown list	Operation mode for scan-analog measurements and peak tasks:
			<ul> <li>SCAN-N (only scan-analog measurements): Ion currents are detected in a mass scan.</li> </ul>
			SCAN-F (only scan-analog measurements):     Ion currents are additionally filtered using a FIR algorithm (FIR: Finite Impulse Response). The filter removes in large part interfering noise from the raw signal of the electrometer preamplifier. Thus, even very small peaks can be detected in the background signal.
			<ul> <li>STAIR-T (only peak tasks): Record a mass spectrum with integer mass jumps.</li> </ul>
			<ul> <li>PEAK-L (only peak tasks):         Scan-analog measurement with         threshold value. Only that peaks         are recorded and displayed, which         exceed the threshold value.</li> </ul>
			<ul><li>PEAK-F (only peak tasks):</li></ul>

			Ion currents are additionally filtered using a FIR algorithm.
•	Detector Type	Dropdown list	Used detector type.
•	Al Channel	Dropdown list	Number of the analog input for measuring data (only relevant for detector type AI in analog input measurement tasks).
•	Gain	Dropdown list	Parameter valid only for QMG700
			Measuring range for the analog input of the QC (only relevant for detector type EXT_IN_# in analog input measurement tasks).
•	SEM Voltage	Number > 0	Operating voltage for the SEM.
			Enter the required value or use the spin buttons.
			The value "0" means that the common SEM voltage is applied. It is displayed and set in the device status view.
•	CP-Level	Number > 0	Parameter valid only for QMG700
			Response threshold of the ion counter preamplifier.
•	Autorange Mode	Dropdown list	In QUADERA®, the amplifier measuring range can be fixed or adjusted automatically.
			FIX:     You can select the measuring range under Amplifier Range.
			<ul> <li>AUTO: The measuring range is selected automatically from all possible ranges.</li> </ul>
			<ul> <li>AUTO-DOWN:         The measuring range is selected automatically from all ranges located between the largest (least sensitive) range and the Range Limit.     </li> </ul>
•	Detector Range	Dropdown list	Measuring range for the ion current (only relevant for Autorange Mode=FIX)
•	Range Limit	Dropdown list	Most sensitive measuring range for the ion current (only relevant for Autorange Mode=AUTO-DOWN)

•	Analog Signal Filter	Dropdown list	Parameter valid only for QMG700  Time constant of analog filter.
•	Resolution	Integer number > 0	Mass resolution (small number = clear separation of peaks). Typical values are approx. 25 for QMG700, and approx. 50 for QMG220.  Enter the required value or use the
•	Pause Calibrate	Number > 0	spin buttons.  A factor used to multiply the pause time determined in the device. In order to wait for transient effects, no measurements are performed during the pause time between two measurement tasks.
			Enter the required value or use the spin buttons.
•	AO Channel	Dropdown list	Number of the analog output.  Measured values are output to this AO.
•	AO Mode	Dropdown list	Parameter valid only for QMG220
			Scales the measurement signal output (010 V). Parameter valid only for specified AO Channel.
•	AO Range	Dropdown list	Parameter valid only for QMG220
			Adjusts the measurement range to the maximum measured signal output. Parameter valid only for specified AO Channel.
•	Trip Type	Dropdown list	Parameter valid only for analog input and total pressure measurement tasks.
			The trip function can monitor measurement values of analog input measurements. Each measurement task provides two trip functions, A and B, and the related threshold values, Level A and Level B. The trip function results are sent to the output Bits DO# A and DO# B.
			• OFF: The trip function is switched off.
			<ul> <li>ABS:         Use the trip function "ABS" for         vacuum monitoring, differential         pressure monitoring, and as         comparator. Read further         information.</li> </ul>

			Use the trip function "HYST" to prevent permanent switching for fluttering signals. Read further information.
•	Level A	Number	Threshold value A (available only for trip types ABS and HYST).
•	DO# A	Integer number > 0	Digital output Bit. The result of the trip function is output to this DO (available only for trip types ABS and HYST).
•	Level B	Number	Threshold value B (available only for trip types ABS and HYST).
•	DO# B	Integer number > 0	Digital output Bit. The result of the trip function is output to this DO (available only for trip type ABS).
•	State	Dropdown list	Status of the measurement task.
			<ul> <li>ENABLE:         The measurement task is being measured and the parameters are being saved.     </li> </ul>
			<ul> <li>SKIP:         The measurement task is not being measured, but the parameters are     </li> </ul>

• HYST:

preserved.

# **Recipe Parameters: MID**

### NOTE:

New or modified parameters for the measurement tasks are accepted by the device only after the measurement has been restarted.

The following recipe parameters are available:

Task Name

<u>Mass</u>

Dwell

**Detector Type** 

**Al Channel** 

Gain (only QMG700)

**SEM Voltage** 

CP-Level (only QMG700)

**Autorange Mode** 

**Detector Range** 

Range Limit

Analog Signal Filter (only QMG700)

**Resolution** 

Pause Calibrate

**AO Channel** 

AO Mode (only QMG220)

AO Range (only QMG220)

Trip Type

Level A

DO# A

Level B

**DO# B** 

**State** 

Parameter		Range	Description
•	Task Name	Letters and digits	Name of the measurement task
•	Mass	Number > 0	Mass number for the measurement task.

			Enter the required value or use the spin buttons.
•	Dwell	Dropdown list	Dwell time for the measurement at the current mass.
			In analog input measurement tasks: Dwell time for the measurement of the analog input of the QC (only relevant for detector type EXT_IN_#).
•	Detector Type	Dropdown list	Used detector type
•	Al Channel	Dropdown list	Number of the analog input for measuring data (only relevant for detector type AI in analog input measurement tasks).
•	Gain	Dropdown list	Parameter valid only for QMG700
			Measuring range for the analog input of the quadrupole controller QC (only relevant for detector type EXT_IN_# in analog input measurement tasks).
•	SEM Voltage	Number > 0	Operating voltage for the SEM.
			Enter the required value or use the spin buttons.
			The value "0" means that the common SEM voltage is applied. It is displayed and set in the device status view.
•	CP-Level	Number > 0	Parameter valid only for QMG700
			Response threshold of the ion counter preamplifier.
•	Autorange Mode	Dropdown list	In QUADERA®, the amplifier measuring range can be fixed or adjusted automatically.
			<ul> <li>FIX: You can select the measuring range under Amplifier Range.</li> </ul>
			<ul> <li>AUTO: The measuring range is selected automatically from all possible ranges.</li> </ul>
			<ul> <li>AUTO-DOWN:         The measuring range is selected automatically from all ranges located between the largest (least sensitive) range and the Range Limit.     </li> </ul>

•	Detector Range	Dropdown list	Measuring range for the ion current (only relevant for Autorange Mode=FIX)
•	Range Limit	Dropdown list	Most sensitive measuring range for the ion current (only relevant for Autorange Mode=AUTO-DOWN)
•	Analog Signal	Dropdown list	Parameter valid only for QMG700
	Filter		Time constant of analog filter.
•	Resolution	Integer number > 0	Mass resolution (small number = clear separation of peaks). Typical values are approx. 25 for QMG700, and approx. 50 for QMG220.
			Enter the required value or use the spin buttons.
•	Pause Calibrate	Number > 0	A factor used to multiply the pause time determined in the device. In order to wait for transient effects, no measurements are performed during the pause time between two measurement tasks.
			Enter the required value or use the spin buttons.
•	AO Channel	Dropdown list	Number of the analog output. Measured values are output to this AO.
•	AO Mode	Dropdown list	Parameter valid only for QMG220
			Scales the measurement signal output (010 V). Parameter valid only for specified AO Channel.
•	AO Range	Dropdown list	Parameter valid only for QMG220
			Adjusts the measurement range to the maximum measured signal output. Parameter valid only for specified AO Channel.
٠	Trip Type	Dropdown list	The trip function can monitor measurement values of MID- and MCD measurements, total pressure measurements, and analog input measurements (AI). Each measurement task provides two trip functions, A and B, and the related threshold values, Level A and Level B. The trip function results are sent to the output Bits DO# A and DO# B.
			• OFF:

The trip function is switched off.

### • ABS:

Use the trip function "ABS" for vacuum monitoring, differential pressure monitoring, and as comparator. Read further information.

## • HYST:

Use the trip function "HYST" to prevent permanent switching for fluttering signals. Read further information.

•	Level A	Number	Threshold value A (available only for trip types ABS and HYST).
•	DO# A	Integer number > 0	Digital output Bit. The result of the trip function is output to this DO (available only for trip types ABS and HYST).
•	Level B	Number	Threshold value B (available only for trip types ABS and HYST).
•	DO# B	Integer number > 0	Digital output Bit. The result of the trip function is output to this DO (available only for trip type ABS).
•	State	Dropdown list	Status of the measurement task.

### • ENABLE:

The measurement task is being measured and the parameters are being saved.

## • SKIP:

The measurement task is not being measured, but the parameters are preserved.

# **Recipe Parameters: MCD**

### NOTE:

New or modified parameters for the measurement tasks are accepted by the device only after the measurement has been restarted.

An MCD measurement project is based on an MID measurement project and includes additional evaluation to yield the components' concentrations of a gas mixture (quantitative gas analysis). Thus, an MCD measurement project always contains a measurement recipe and an analysis matrix which contains the gas specific calibration factors. The MCD measurement project is closely related to a gas specific calibration which is needed to determine the relevant calibration factors. Note that you should perform the gas specific calibration directly before the MCD measurement project.

## **Analysis matrix (MCD Matrix Editor)**

The analysis matrix connects the MID measurement recipe with the gas components:

- The rows of the analysis matrix are defined by the name of the gas components for the quantitative analysis.
- Use the "Add MCD Task" tool to add a row (gas component) to the matrix.

#### NOTE:

In the MCD project, use identical names for the gas components as used in the gas specific calibration. Otherwise, QUADERA® cannot refer to the components. As an example, QUADERA® does not equate "O2" and "Oxygen".

- The columns of the analysis matrix are defined by the measurement recipe, and correspond to the mass numbers in the measurement tasks.
- The individual matrix elements represent the gas specific calibration factors for the quantitative gas analysis. The calibration factors are determined in the gas specific calibration and stored in the MCD Calibration Factor Library.

# **Recipe Parameters: Total Pressure**

This chapter is valid for the QMG220 only.

### NOTE:

New or modified parameters for the measurement tasks are accepted by the device only after the measurement has been restarted.

The following recipe parameters are available::

Task Name

<u>Dwell</u>

**Detector Type** 

Trip Type

Level A

<u>DO# A</u>

Level B

<u>DO# B</u>

<u>State</u>

Parameter	Range	Description
Task Name	Letters and digits	Name of the measurement task.
• Dwell	Dropdown list	Dwell time for the measurement of the total pressure.
<ul><li>Detector Type</li></ul>	(not editable)	Detector type "TotalPressure": installed total pressure gauge
• Trip Type	Dropdown list	The trip function can monitor measurement values of total pressure measurements. Each measurement task provides two trip functions, A and B, and the related threshold values, Level A and Level B. The trip function results are sent to the output Bits DO# A and DO# B.
		<ul> <li>OFF: The trip function is switched off.</li> </ul>
		<ul> <li>ABS:         Use the trip function "ABS" for         vacuum monitoring, differential         pressure monitoring, and as         comparator. Read further</li> </ul>

## information.

### • HYST:

Use the trip function "HYST" to prevent permanent switching for fluttering signals. Read further information.

•	Level A	Number	Threshold value A (available only for trip types ABS and HYST).
•	DO# A	Integer number > 0	Digital output Bit. The result of the trip function is output to this DO (available only for trip types ABS and HYST).
•	Level B	Number	Threshold value B (available only for trip types ABS and HYST).
•	DO# B	Integer number > 0	Digital output Bit. The result of the trip function is output to this DO (available only for trip type ABS).
•	State	Dropdown list	Status of the measurement task.

#### Status of the measurement i

### • ENABLE:

The measurement task is being measured and the parameters are being saved.

## • SKIP:

The measurement task is not being measured, but the parameters are preserved.

## **Trip Function ABS**

Use the trip function "ABS" for the following purposes:

- <u>Vacuum monitoring</u>,
- <u>Differential pressure monitoring</u>,
- Windows comparator.

## Vacuum monitoring

Requires just the trip function Trip A. Proceed as follows to use the trip function for vacuum monitoring in MID and MCD measurement projects:

- 1. Select trip type "ABS".
- 2. Enter the threshold value "Level A".
- 3. Set the digital output Bit "DO# A". The result of the trip function is output to DO# A.

The trip function ABS-Trip A switches on when the signal falls below Level A.



### Differential pressure monitoring

Requires just the trip function Trip B. Proceed as follows to use the trip function for differential pressure monitoring in MID and MCD measurement projects:

- 1. Select trip type "ABS".
- 2. Enter the threshold value "Level B".
- 3. Set the digital output Bit "DO# B". The result of the trip function is output to DO# B.

The trip function ABS-Trip B switches on when the signal exceeds Level B.

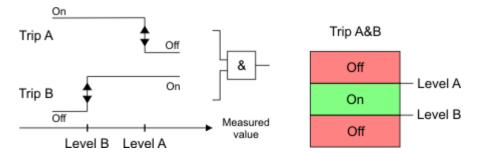


### **Windows Comparator**

Requires the two trip function Trip A and Trip B. Proceed as follows to use the trip functions as comparator in MID and MCD measurement projects:

- 1. Select trip type "ABS".
- 2. Enter the upper threshold value "Level A".
- 3. Enter the lower threshold value "Level B".
- 4. Set identical values to the digital output Bits "DO# A" and "DO# B", i.e. DO# A: xx and DO# B: xx. The two trip functions are conjoined (logical operator AND).

The trip function ABS switches on when the signal is in the range between the threshold values Level B and Level A.



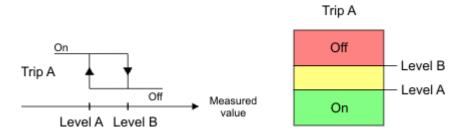
# **Trip Function HYST**

Use the trip function "HYST" (hysteresis) to prevent permanent switching for fluttering signals.

This requires just the trip function Trip A. Proceed as follows to use the hysteresis trip function "HYST" in MID and MCD measurement projects:

- 1. Select trip type "HYST".
- 2. Enter the lower threshold value "Level A".
- 3. Enter the upper threshold value "Level B".
- 4. Set the digital output Bit "DO# A". The result of the trip function is output to DO# A.

The trip function HYST switches on when the signal falls below Level A, and it switches off when the signal exceeds Level B.



# **Processing Measurement Data**

## Minimum

### Action

Return the smallest measuring value found in the selected part of the measuring curve:

```
\begin{aligned} & \text{Minimum} &= \text{Minimum}(x_1, \ x_2, \ \dots, \ x_n), \\ & x_1 \ \dots \ x_n &= \text{Measuring values 1} \ \dots \ n \ \text{in the selected part} \end{aligned}
```

# **Average**

### Action

Calculate the average value for all measuring values located in the selected part of the measuring curve:

Average = 
$$\frac{\sum X_i}{n}$$
,

 $x_i$  = Measuring value; n = number of measuring values in the selected part

## Maximum

### Action

Return the largest measuring value found in the selected part of the measuring curve:

```
\begin{aligned} & \text{Maximum} = \text{Maximum}(x_1, \ x_2, \ \dots, \ x_n), \\ & x_1 \ \dots \ x_n = \text{Measuring values 1} \ \dots \ n \ \text{in the selected part} \end{aligned}
```

## **Absolute Standard Deviation**

### Action

Calculate the absolute standard deviation for all measuring values located in the selected part of the measuring curve:

$$\mathsf{STDABS} = \sqrt{\frac{\sum \chi_i^2 - n \cdot \mathsf{Average}^2}{n - 1}},$$

 $x_i$  = Measuring value; n = number of measuring values in the selected part

# **Automating Tasks**

## Triggered Run Add-in

The purpose of the Triggered Run Add-in (installed with QUADERA 4.40) is to provide a QUADERA Add-in that automates the execution of multiple QUADERA operations. These operations include loading a Template, running the associated Measurement Project, saving its data, and then exporting that data into an ASCII file. These operations are combined into what is referred to as a Triggered Run Task. The Add-in has the ability to create and configure a list of these tasks prior to run time. The Add-in also manages configuration of the execution of this task list by means of digital input triggering.

The Add-in provides the following functionality:

- Allows multiple Triggered Run Tasks, where each task can be configured so that:
  - A Template can be selected.
  - The Save Files can be defined. (Save file is of type .qmp, and the exported ASCII file will have the same name, with the .asc extension.)
  - The Filament can be turned on or off.
  - The SEM can be turned on or off.
- Allows the user to select the desired QMG device.
- Allows the user to select the Digital Input to be used as the Trigger.
- Allows the user to select the how the Digital Input should be used:
  - The QMG can run when the Digital Input switches on and then stop when it switches off.
  - The QMG can run when the Digital Input switches off and then stop when it switches on.
- Allows automatic preparation of the system, so that all Measurement Files have been opened and the QMG is ready to run.
- Allows the user to begin watching for triggers.
- Allows the user to stop watching for triggers.
- Requires user approval prior to exporting data.
- Automatically manages switching through the list of Tasks.
- Allows the user to save all configuration information.

This sequence of steps should be followed to run the Triggered Run Add-in:

• Select QMG – In the list labeled "Select QMG" choose the QMG to be used for the run. Only one QMG can be selected for a run.

- Configure the Task List A Task is an operation that uses a given template to open a Measurement File, configures the QMG Filament and SEM, runs that QMG and then finally saves and exports the associated data.
  - Add New Using the text boxes under the list view, define the parameters of a new Task.

•

- Template Enter the name of an existing template stored in the default template directory, including .qmt extension, or use the browse button to navigate to the desired template.
- Save As Enter in the name to give the saved Measurement File, including extension .qmp. This entered File name will also be used to save the exported ASCII file, but it will use the .asc extension instead.
- Filament Check "Filament" if it is desired for this task to be run with the filament turned on.
- SEM Check "SEM" if it is desired to run this task with the SEM turned on.
- Click "Add Task" and a new row will be added to the table with the parameters as defined above.
- Update Task When a task is selected in the table, the fields for editing are automatically filled. The user can modify any or all of the fields and then click the "Update Task" button. The selected row will be updated with the new values.
- Delete Task When one or more rows are selected in the table, and the "Delete task" button is clicked, those rows will be removed.
- No changes are saved until the "Save" button is clicked or "Ok" is used to dismiss the dialog.
- Configure the Run The Run (i.e. how all tasks will be executed) can be configured by the controls in the group labeled "Manage Running of Tasks".
  - Connect Connect executes the task of making a connection between QUADERA and the QMG device. You must connect prior to configuring the Run. Certain information is only available after connection. If the Button says "Connect" then you must connect to the selected QMG. If the button says "Disconnect" then the QMG is already connected and you are ready to configure.
  - "Run while DI On" indicates that the user wants each task to start and run
    when the Digital Input indicated changes state to "On" (if checked) or "Off" (if
    not checked).
    - If "Run while DI On" is checked, then when the Digital Input changes to "On", the next task will begin running. When that Digital Input changes to "Off", it will stop the task from running.
    - If "Run while DI On" is not checked, then when the Digital Input changes to "Off", the next task will begin running. When that Digital Input changes to "On", it will stop the task from running.
  - "Run while DI On" is used for immediately starting the run if the start condition is true. After clicking the "Start" button, the run will begin with out waiting for a change in the Digital Input.
  - "Digital Input to watch" is a list ranging from 1 to the number of Digital Inputs in the QMG device This indicates which Digital Input will be used as the trigger for the run.

- "Reload when Finished" indicates that the scheduled run will be reloaded after completing the previous run. The next run is loaded, but it will not start watching for triggers until the "Start" button has been clicked. The next set of files will have their name appended with an index "(#)". This will increment and the runs will continue reloading until the Add-in has been dismissed.
- "Restart after Reload" will be enabled if "Reload when Finished" has been checked. Using "Restart after Reload" skips the need for the user to click on "Start" after each run. The Add-in will immediately begin watching for triggers as soon as it has completed reloading.
- "Start" Click "Start" after both the tasks and the Run have been configured. This will tell the Add-in to begin loading Measurement Files and to prepare for the Run. The Add-in will begin watching for value changes on the selected Digital Input. When that Digital Input changes value it triggers the Add-in to take action by either starting or stopping the current Task. By using these Triggers, the Add-in starts and stops each Task, iterating through the list until they have all been executed.
- "Stop" Once the "Start" button has been clicked, the button text will change to "Stop". Clicking the button at this point will manually stop the run.
- Completion of the run When the run has been completed, the Add-in will automatically save the data file and export the data.

# Scripting

## **Scripting**

Scripting has been integrated into the host application, enabling the user to adapt the functions of the application to his or her needs. Scripting always requires the host application in order to be executed.

The Visual Studio Tools for Applications (VSTA) development system is suited to customize applications by using the .NET framework. VSTA replaces Visual Basic for Applications (VBA) and uses Visual Studio as the IDE.

With scripting, you can develop your own solutions to problems and in this way automate and extend the functions of the application. You can develop solutions that extend the functions of your application and that may be used again and again. By integrating VSTA, QUADERA® provides the user with a widely used and supported programming environment.

## **Scripting within QUADERA®**

QUADERA® stores scripting code in a main <u>scripting directory</u>. The individual modules (add-ins) are stored separately. When required, the add-ins are available for all measurement project templates.

QUADERA® provides examples for add-ins and measurement project templates that use these Add-ins. You can use the templates via the <u>start page</u>.

#### NOTE:

For further information on scripting and the programming environment, please refer to the help file for Microsoft Visual Studio Tools for Applications. Use the Help menu of the VSTA editor.

### NOTE:

The <u>help system for the scripting functions</u> within QUADERA® explains the extended instruction set and the corresponding syntax.

### NOTE:

The QUADERA® Release Notes ("Readme.html" file) provide a description of "Saving VBA code for reprogramming in VSTA" to support users who have been working with VBA up to now.

# **Scripting Directory Structure**

### File types

A scripting add-in contains the following file types:

- Add-in DLL:
   .Net assembly which contains the compiled add-in code (\*.dll),
- Source code:
   These are the files which allow the user to view, edit and compile the add-in. The main file is a "Visual Basic .Net" project (\*.vbproj) which then contains links to other files such as VB.Net code (\*.vb).

#### **Directories**

Scripting add-ins are stored by default in the directory "My Documents\My Quadera\Scripting":

- The sub-directory "MeasureProjectAddIns" contains the add-in DLL Files,
- The sub-directory "Code" contains the source code files. Each add-in is stored in a separate directory.

Add-ins which are present in the "MeasureProjectAddIns" directory can be used by QUADERA and will be listed in the "Add-in Manager" dialog. An add-in does not need to have source code available. However, without this the user will be unable to view or edit the code.

### Example

The following table shows an example file structure for an add-in with the name "Sample":

(directories appear in normal type, files in italics)

⁄ S∈	cripting	
		♦ Sample.dll
		♦ Sample.vbproj
		♦ ThisMeasureProject.vb
		♦ <other code<br="" source="">files&gt;</other>

Note that you can change the <u>file location of the scripting directory</u>.

# **Copying Add-ins**

Proceed as follows to copy an add-in:

- 1. Copy the add-in DLL file to the "MeasureProjectAddIns" directory.
- 2. If source code is also available:
  - a. Create a new directory under "Code" with the name of the add-in (without the DLL extension!).
  - b. Copy the source code files to this directory.

# **Deleting Add-ins**

## NOTE:

Add-ins can be used by more than one measurement project. Care should be taken when deleting an add-in.

Proceed as follows to delete an add-in:

- 1. Remove the add-in DLL file from the "MeasureProjectAddIns" directory.
- 2. If source code is also available: Remove the directory with the add-in name from the "Code" directory.

# **Using Macros**

## **Creating Add-ins and Macros**

In VSTA, an add-in can include more than one function. Each function can be considered as a macro and an add-in as "macro collection". Thus, you have two options to create a new macro:

- Edit an existing add-in to include a new function that can be used as macro,
- Create a new add-in and program a function that can be used as macro.

The following steps describe how to create a new add-in.

- 1. Open an existing measurement project, or create a new measurement project.
- 2. In the Tools menu, point to Programming.
- 3. In the submenu, select **Create Add-in...** The "Create Add-in" window opens up.
- 4. Use the field to specify the name of the add-in.
- 5. Click [OK]. The VSTA editor opens up. Now you can create the new add-in:
  - VSTA automatically creates the basic structure of the add-in that is executable without any functions,
  - Then you can program your own functions to expand the add-in.

QUADERA® stores each add-in in a main <u>scripting directory</u>. When required the add-ins are available for all measurement project templates.

#### NOTE:

For further information on scripting and the programming environment, please refer to the help file for Microsoft Visual Studio Tools for Applications. Use the Help menu of the VSTA editor.

# **Activating Add-ins**

- 1. Open an existing measurement project, or create a new measurement project.
- 2. In the **Tools** menu, point to **Programming**.
- 3. In the submenu, select **Add-in Manager...**. The "Add-in Manager" window opens up.
- 4. In the displayed "Available Add-ins" list, enable the checkbox next to the name of the required add-in.
- 5. Click **[OK]**.

# **Running Macros**

### **Automatic run**

QUADERA® automatically executes macros in the following cases:

- An add-in is loaded and its startup code calls up the macro,
- A QUADERA® event calls up the macro.

### Manual run

You have to activate the relevant add-in before you can manually execute the macro.

- 1. In the **Tools** menu, point to **Programming**.
- 2. In the submenu, select **Macros...**. The "Macros" window opens up.
- 3. In the displayed macro list, click the name of the macro to be executed (not the checkbox).
- 4. Click Run.

## NOTE:

You can call up the "Macros" window with the keyboard shortcut ALT+F8.

# **Editing Add-ins and Macros**

In VSTA, an add-in can include more than one function. Each function can be considered as a macro and an add-in as "macro collection". Proceed as follows to edit an add-in or an included macro:

- 1. Open an existing measurement project, or create a new measurement project.
- 2. In the Tools menu, point to Programming.
- 3. In the submenu, select **Add-in Manager...**. The "Add-in Manager" window opens up.
- 4. In the displayed "Available Add-ins" list, click the name of the add-in to be edited, or browse for the required add-in.
- 5. Click [Edit]. The source code will then be opened in the VSTA editor for editing.

QUADERA® stores each add-in in a main <u>scripting directory</u>. When required, the add-ins are available for all measurement project templates.

### NOTE:

For further information on scripting and the programming environment, please refer to the help file for Microsoft Visual Studio Tools for Applications. Use the <u>Help menu of the VSTA editor</u>.

# Calling Up the VSTA Editor

- 1. Open an existing measurement project, or create a new measurement project.
- 2. In the **Tools** menu, point to **Programming**.
- 3. In the submenu, select **Add-in Manager...**. The "Add-in Manager" window opens up.
- 4. In the displayed "Available Add-ins" list, click the name (not the checkbox) of the add-in to be edited, or browse for the required add-in.
- 5. Click [Edit]. The source code is being opened in the VSTA editor for editing.

QUADERA® stores each add-in in a main <u>scripting directory</u>. When required the add-ins are available for all measurement project templates.

#### NOTE

For further information on scripting and the programming environment, please refer to the help file for Microsoft Visual Studio Tools for Applications. Use the Help menu of the VSTA editor.

# Calling Up the VSTA Help

- 1. Call up the VSTA editor. (e.g. Edit an available Add-in).
- 2. In the **Help** menu, select the required item.

or

2. Press the **F1** key.

#### NOTE

The VSTA Help includes the help for the specific <u>QUADERA® scripting</u> <u>functionality</u>.

# **Spectra Library**

# **Spectra Library**

A Spectra Library is available for comparison of device spectrum to compound spectra.

The Spectra Library is accessed via the Tools>>Spectra Library menu selection or from any Bargraph Cycles measurement project.

The Spectra Library view and contents can be customized and saved.

# Operating the Input/Output Module

- Quadrupole mass spectrometer QMG220: input/output module IO220
- Quadrupole mass spectrometer QMG700: input/output module IO700

# **ACAUTION**



Setting digital and analog output values.

Improper operation of the input/output module by setting incorrect digital and analog output values can damage the device.

Only trained service personnel and personnel with similar training may set the digital and analog output values of the input/output module.

Use the relevant <u>measurement project</u> as a user interface for testing and servicing the input/output module (if existing). For this, connect the device with QUADERA®.

- Digital Inputs: display the states of the digital input (DI) channels:
  - Number: identification of the DI channel,
  - Value: value of the DI channel (On/Off),
- Digital Outputs: switch on and off the digital output channels (DO) manually:
  - Number: identification of the DO channel,
  - Value: value of the DO channel (On/Off),
- Analog Inputs: display the voltage at the analog input (AI):
  - Number: identification of the AI channel.
  - Value: numerical value of the voltage at the AI channel.

Add a measurement task "Add Analog Input Task" to Scan and MID measurement projects to measure the voltage at a analog input.

- Analog Outputs: Change the voltage at the analog output (AO):
  - Number: identification of the analog output,
  - Value: numerical value of the voltage at the analog output.

# **Creating IO Characteristics**

# **Creating Input/Output Characteristics**

Characteristics can be created for Analog Inputs and Outputs. Characteristics can be assigned to one or all devices. Analog I/O Characteristics work with the following devices:

- Quadrupole mass spectrometer QMG220: input/output module IO220
- Quadrupole mass spectrometer QMG700: input/output module IO700

The Characteristics Editor can be accessed from the context-menu of the All Device Status View or from the Device Configuration.

Characteristics can be saved to the software device in QUADERA® from a Measurement Project.

The function of AI/AO Characteristics allows definition of a characteristic set of data that can be applied to an Analog Input or Analog Output. Once defined, these characteristics are then available for use on any Analog Input or Output. For example, a set of data can be defined that produces a charted temperature for an Analog Input.

Example: X\*1.8 + 32

The AI/AO Characteristics dialog can be accessed from the Tools>> AI/AO Characteristics menu selection. From this dialog new Characteristics can be created and edited. Characteristics can also be copied (to create a new Characteristic from a standard Characteristic) or deleted. The Characteristic Definition Editor provides a table, graph and formula interface for easy creation of the Characteristic. The Definition Editor is also where the Characteristic type is defined – Analog Input, Analog Output or Analog Input to Analog Output. A name and unit must also be entered in this editor.

The formula interface describes the Y value as a function of X. The formula can use the operators of + - \* / ^ as well as the following functions:

Description	Enter as:	Mathematical Equivalent
Calculation of e to the power of X	exn(X)	e^X
Calculation of 10 to the power of X	exp(X)	10^X
Calculation of the	lgn()	In()

logarithm, base e		
Calculation of the logarithm, base 10	log()	lg()
Squared	sqr()	X^2
Calculation of the square root	srt()	X^(1/2)
Determination of the absolute value	abs()	X
Trigonometric functions	Sin(),Cos(),Tan()	Sin(),Cos(),Tan()
Expressions in parentheses	( )	( )
Pi	Pi	Pi

The formula parser will indicate when a formula is constructed incorrectly. Note that the parser may indicate 'Operator Input Error' as the formula is being entered. Disregard that message unless it appears when the formula is finalized.

AI/AO Characteristics are then assigned to Analog Inputs and Analog Outputs via the context menu item 'AI/AO Characteristics' in any MID chart. Once a Characteristic is assigned to an Analog Input it is used for that Analog Input in any MID Measurement Project that uses that Analog Input. For example, if Analog Input 1 is wired to a temperature sensor, and a Characteristic is assigned to Analog Input 1, then all MID Measurement Projects that use Analog Input 1 will automatically use that Characteristic.

# Warning and Error Messages

# **List of Events**

The event view informs you on the occurred events:

- "Date/Time" displays the time when the event occurred,
- "Source" displays the source that caused the event, e.g. measurement or device,
- "Type" displays the event type ("Information", "Warning", "Error"),
- "Description" displays a brief message text on the event, and specifies warnings and errors. This three-part specification contains:
  - the device specification,
  - the code letter of the event type ("E" means error, "W" means warning),
  - the three-digit identification number of the event.

## List of events sorted by identification numbers:

- Warning messages ("W") for the QMG220:
  - W001: "emission current out of tolerance"
  - W002: "emission current wide out of tolerance"
  - W003: "RF-stage temperature is high"
- Error messages ("E") for the QMG220:
  - E001: "external protection triggered"
  - E002: "emission error"
  - E003: "filament 1 defect"
  - E004: "filament 2 defect"
  - E005: "RF-stage switched off because of excessive temperature"
  - E009: "ionsource error"
  - <u>E039</u>: "SEM error"

# Warning Messages for the QMG220

# Warning Message QMG220.W001

## Message text:

"emission current out of tolerance"

### **Description:**

The emission current deviates from the set value.

### Message occurs when?

• The emission current deviates 10% and more than 40  $\mu A$  from the specified value.

### Reasons

- The emission current control is faulty,
- The pressure in the recipient is unstable.

## Consequences

• Measuring data are corrupt.

### **Solutions**

• Replace the IS220 when the message occurs repeatedly with stable pressure conditions.

# Warning Message QMG220.W002

## Message text:

"emission current wide out of tolerance"

## Description:

The emission current essentially deviates from the set value.

## Message occurs when?

• The  $\underline{\text{emission current}}$  deviates more than 20% and more than 40  $\mu\text{A}$  from the specified value.

#### Reasons

- · The emission current control is faulty,
- The pressure in the recipient is unstable.

## Consequences

Measuring data are corrupt.

### **Solutions**

 Replace the IS220 when the message occurs repeatedly with stable pressure conditions.

# Warning Message QMG220.W003

#### Message text:

"RF-stage temperature is high"

### **Description:**

The temperature of the RF stage has exceeded 65°C.

### Message occurs when?

• The temperature of the RF stage exceeds 65°C.

#### Reasons

- Cooling of the RF stage is not sufficient because the fan filter pad is blocked,
- The fan is defective.

### Consequences

• Measuring data are corrupt.

- Check the fan filter pad,
- Repair the fan.

# **Error Messages for the QMG220**

### Error Message QMG220.E001

#### Message text:

"external protection triggered"

#### Description:

The protection for SEM and filament has triggered.

### Message occurs when?

- The specified threshold is exceeded when monitoring the total pressure,
- The external protection is triggered,
- The total pressure gauge is not properly connected, or the protection input is not properly connected.

#### Reasons

- Connected total pressure gauge: the pressure has exceeded the specified threshold,
- The total pressure gauge reports an error,
- The total pressure gauge is defective or disconnected,
- The total pressure gauge is switched off.

#### Consequences

• Filament and SEM are switched on and off depending on the selected protection mode.

- Set the protection mode to internal protection.
- · Connect a total pressure gauge.
- Modify the threshold of the total pressure gauge.

#### Message text:

"emission error"

### **Description:**

An emission error occurred.

### Message occurs when?

- The specified emission current is not reached,
- The <u>protection current</u> for the filament is triggered.

#### Reasons

• The filament emission current is too low.

### Consequences

- Ionization is impossible,
- Measuring data are not meaningful.

- Check the specified protection current for the filament,
- Replace the filament. Refer to the device specific instructions of the QMG (OEM manual) for further information,
- Switch over to the other filament (when existing).

### Message text:

"filament 1 defect"

## **Description:**

The filament 1 is broken.

### Message occurs when?

- A broken filament is detected when the device is switched on,
- A broken filament is detected when the filament is switched on,
- The filament is missing.

#### Reasons

• The filament is defective.

### Consequences

- Ionization is impossible,
- The filament can not be switched on,
- Measuring data are not meaningful.

- Replace the filament. Refer to the device specific instructions of the QMG (OEM manual) for further information.
- <u>Switch over to the filament 2</u> (when existing).

### Message text:

"filament 2 defect"

## **Description:**

The filament 2 is broken.

### Message occurs when?

- A broken filament is detected when the device is switched on,
- A broken filament is detected when the filament is switched on,
- The filament is missing.

#### Reasons

• The filament is defective.

### Consequences

- Ionization is impossible,
- The filament can not be switched on,
- Measuring data are not meaningful.

- Replace the filament. Refer to the device specific instructions of the QMG (OEM manual) for further information.
- <u>Switch over to the filament 2</u> (when existing).

#### Message text:

"RF-stage switched off because of excessive temperature"

### Description:

The RF stage was switched off because the temperature has exceeded 80°C.

### Message occurs when?

• The temperature of the RF stage exceeds 80°C.

#### Reasons

- Cooling of the RF stage is not sufficient because the fan filter pad is blocked,
- The fan is defective.

### Consequences

- The power supply of the RF stage is switched off,
- Measuring data are not meaningful.

- Check the fan filter pad,
- · Repair the fan,
- Switch the device off, and wait until the RF stage has cooled down. Then switch the device on again.

### Message text:

"ionsource error"

### **Description:**

An error occurred in the power supply of the ion source.

### Message occurs when?

- The current related to the ion reference voltage is too high,
- The current limit is exceeded in degas mode,
- The power supply of the IS220 is not ok.

#### Reasons

- The feeder of the IS220 is not ok,
- The connected ion source is short-circuited,
- The specified protection current limit for degas mode is too low.

#### Consequences

- The ion source is operating faulty,
- Measuring data are not meaningful.

- · Check and correct contacts and cable of the IS220 power supply,
- Dismount the ion source. Clean or repair it,
- Increase the protection current for degas mode.

### Message text:

"SEM error"

## **Description:**

An error occurred in the control of the SEM voltage.

### Message occurs when?

- The <u>SEM voltage</u> deviates 10% and more than 30 V from the specified value,
- In case of a short circuit.

#### Reasons

• The SEM is contaminated or defective.

### Consequences

- The SEM switches off,
- Measuring data are not meaningful when using the SEM.

#### **Solutions**

• Check the SEM. Refer to the device specific instructions of the SEM (OEM manual) for further information.

# **Scripting in QUADERA**

#### NOTE:

You first have to activate the QUADERA® VSTA functionality through an appropriate license key in order to use 'scripting'. Adhere to the notes given in the Release Notes and to the "About..." dialog.

You can use the VSTA functions provided by QUADERA® to automate tasks and to tailor them according to your needs. The available instructions, how to use them, and the syntax is integrated into the Help of the VSTA editor:

- Open the VSTA editor,
- Open the object browser (menu View > Object Browser),
- Open the library "Quadera",
- · Click on the required component,
- The bottom right part of the window displays the available information on the component. Press the **F1** key to invoke the general VSTA Help.

NOTE: QUADERA® provides examples for add-ins and measurement project templates that use these Add-ins. You can use the templates via the <u>start page</u>.

NOTE: VSTA Add-ins can be started from the QUADERA command line if desired. There is a command line option – [/addin] that can be used with the Add-in name. As an example (XP English shown), the following command line can be used to automatically load and start the [GSD320] Add-in:

C:\Program Files\QUADERA\Quadera.exe /addin:GSD320

To modify the command line, create a program shortcut in Windows and edit the shortcut's Properties>>Target field.

# **Glossary**

# A

AI: Analog Input: Analog (continuous) input of the mass spectrometer.

amu: atomic mass unit.

Analog Input: Analog (continuous) input of the mass spectrometer.Analog Output: Analog (continuous) output of the mass spectrometer.AO: Analog Output: Analog (continuous) output of the mass spectrometer.

# В

**Background:** See Mass spectrometer background.

Bar graph: Display of measuring data on a category axis.

**Button:** Graphical representation of a binary switch.

# C

**C-SEM:** Secondary electron multiplier with channeltron (also known as channel electron multiplier).

Category: In QUADERA: A non-continuous division of a measuring data axis.

**Context menu:** A context menu can be called up by clicking certain spots in the graphical user interface with the right mouse button. It contains only menu items that make sense in the clicked area (object specific functions).

# D

**Data navigator:** Operating element for navigation within the measuring data. The data navigator is especially useful when handling large amounts of data.

**Degassing:** For a specified time, the filament receives a current that is higher than usual. This heats out the measuring head and cleans it from contamination.

**DI:** Digital Input: Digital (binary) input of the mass spectrometer.

**Digital Input:** Digital (binary) input of the mass spectrometer.

**Digital Output:** Digital (binary) output of the mass spectrometer.

**Dimension:** Relation between a quantity of physics and the basic quantities.

**DO:** Digital Output: Digital (binary) output of the mass spectrometer.

# Ε

**Emission current:** Electron current required for ionizing the analysis gas.

**Event display:** Display for events: Warnings, informations, errors.

F

**Filament:** Glowing wire which emits the electrons required for ionizing the gas molecules.

FIR: Finite Impulse Response (digital filter).

G

**Gas specific calibration factors:** Correction factors, used for calculating partial pressures from ion currents.

**Graphics:** Display with a graphical representation of the measuring values (line graph, bar graph, ...).

**GSC:** Gas Specific Calibration.

Н

**Hold:** Used if data are being analyzed while a measurement is running. The command freezes the section it its current state (the latest measuring data are not being displayed). However, the measurement continues in the background.

I

**Ion source optimization:** Calibration process during which the ion source is adjusted in order to optimize the ion current with respect to the intensity and/or the peak shape.

# M

**Mass scale calibration:** Correction between nominal mass number and actual peak maximum.

**Mass spectrometer background:** Background determination by the software. Mostly, a zero gas is used for this.

**MCD:** Multiple Concentration Determination. In this measuring mode, the concentration of the individual gas components is calculated from measured ion currents.

**Measurement project:** Contains all instruments required to perform a specific measurement task. One device is assigned to each measurement project. It is possible that several measurement projects relate to the same device.

Measurement project template: See Template.

**Measurement task:** Constitutes the basic component of a recipe and contains the measuring mode and all parameters required to specify this mode. Measurement tasks can be configured.

Measuring mode: The different types of measurement that are supported by the device.

**MID:** Multiple Ion Detection. In this measuring mode, the intensity for specified masses is measured as a partial pressure or ion current.

**MS**: Mass spectrometer.

N

**Nominal mass:** Expected mass of an element.

O

**Object:** General term for elements that are being used in the software in any way, e.g. chart, task.

**Offset:** Offset of a real measuring amplifier from zero.

P

**Parameter set:** Group of parameters that are related or belong together otherwise (settings).

**Partial pressure:** Pressure that is being created by an individual component in a gas mixture.

**Peak:** A scan-analog spectrum consists of a number of peaks. These represent fractions of the individual gas components at the respective masses.

**PGA:** Process gas analysis.

**ppb:** Parts per billion (1 : 1,000,000,000).

**ppm:** Parts per million (1 : 1,000,000).

**Process gas analysis:** Analysis of gas mixtures that are being expected in a process.

Property dialog field: Dialog window, generally containing several tabs.

Q

**QC:** Quadrupole Controller. See operating instructions QMG.

QMG220: High-end mass spectrometer.

**QMG700:** High-end mass spectrometer.

QUADERA: Operation and analysis software for the QMG mass spectrometers.

R

**Recipe:** A recipe is a sequence of measurement tasks.

**RF:** Radio Frequency.

**RGA:** Residual Gas Analyzer.

S

Scan: See Scan Analog.

**Scan Analog:** Ion current as a function of m/e.

Scan speed: Sampling rate for scan-analog measurements. In most cases the time/mass.

**Scan-F filter:** FIR filter, used for smoothing a scan-analog signal.

**Scripting:** Programming of specific routines. In QUADERA, scripting has been implemented with VSTA.

**Section:** Part of the working area. Any working area can be divided into so-called sections by the user. Each section can be filled with a graphical object (e.g. measuring data display).

SEM: Secondary Electron Multiplier.

**Sensitivity:** The sensitivity is the basis to calculate partial pressures from ion currents. The sensitivity is used together with the gas specific calibration factors, and can be determined from measurements.

**SEV:** Sekundärelektronenvervielfacher (German expression for SEM).

**SPM:** Sputter Process Monitor.

Т

**Template:** Predefined settings which help the user to create a measurement project (configuration of the measurement without measuring data).

**Toolbox:** Graphical operating element which depicts functions with small pictograms. The functions are activated or executed by dragging & dropping the related pictograms.

**Trend:** Course of a value with time.

Trend display: Graphical display for the course of a measured quantity with time.

**Tune Mode:** Procedure for tuning a device such as the ion source and optimizing the signal shape.

U

**Unit:** Quantity of physics = Numerical value \* unit.

V

**VBA:** Visual Basic for Applications. Scripting language by Microsoft which is used for programming in applications. Followed by VSTA.

**VSTA:** Visual Studio Tools for Applications. Development system to customize applications by using the .NET framework. Replaces VBA.

W

**Working area:** Part of the measurement project window or recipe. The working area is used to display measuring data or to specify parameters for the currently selected recipe.

Workspace: See Working area

**WYSIWYG:** "What You See Is What You Get": The displayed screen is being output at the printer as faithfully as possible.

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