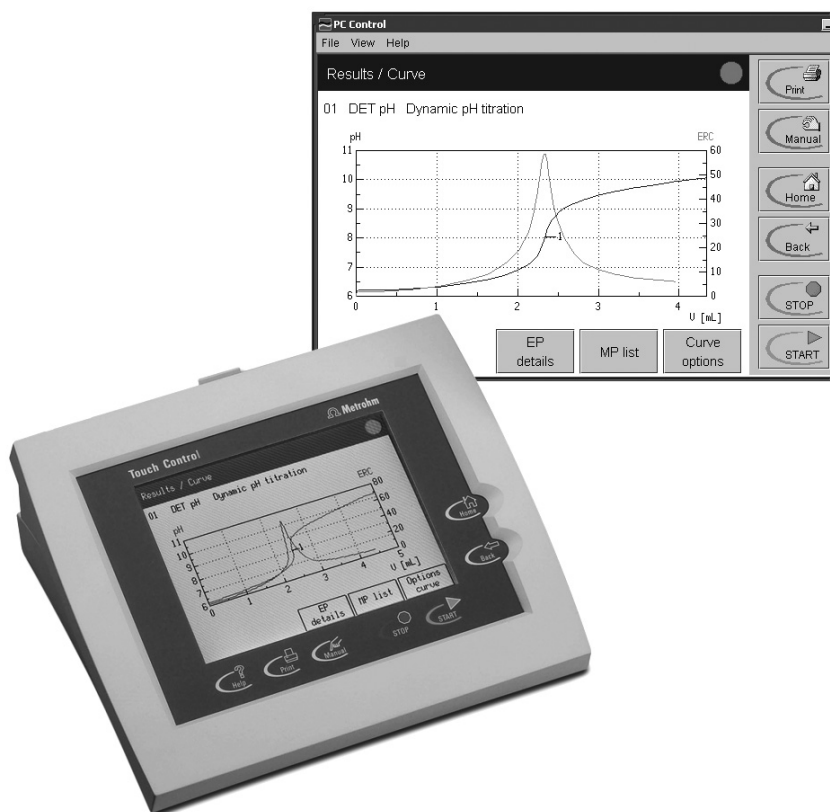


PC Control / Touch Control



Manual
8.840.8003EN



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PC Control Touch Control

Program version PC Control 5.0
Touch Control 5.840.0140

Manual

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Although all the information given in this documentation has been checked with great care, errors cannot be entirely excluded. Should you notice any mistakes please send us your comments using the address given above.

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1 Introduction

This manual gives you a comprehensive overview of the functions of the **Touch Control** and the **PC Control** software for operating the Titrand system. The Titrand system can either be operated with the **Touch Control with touch-sensitive screen** as a stand-alone-system or with the PC software **PC Control**. In this case the varied possibilities of a computer can be utilized.

Figure 1.1 shows the versatility of the Titrand system. On the left a Touch Control for operating a Titrand with external dosing devices is shown. To the right you can see an automation system consisting of USB Sample Processor, Titrand with internal dosing drive and Dosimat controlled by the PC Control software.



Fig. 1.1: The Titrand system

1.1 Instrument description

There are two different ways of operating the Titrando system: with **Touch Control** the operation is via a touch-sensitive screen. A computer with installed **PC Control** software is a version with several additional features which directly utilize the communications and storage facilities of a PC. The import of Titrino methods is only possible with the PC Control software. Both programs have a context-sensitive **online help** function.

The appearance and operation of the two versions are almost identical; this means that if you work with Touch Control then you can also use the PC Control software without any problems and vice-versa. Methods, determinations, sample data silos, result silos and backups are **100 % compatible**.

This manual describes the operation of the Titrando system with both the PC Control software and Touch Control. If the description applies to only one of these versions then this is indicated in the text.

Further documents can be found on the installation CD of PC Control. Visit the web page <http://products.metrohm.com> as well. There you will always find the most recent documents ready for download as PDF files.

1.2 About the documentation







Attention!

Please read through this documentation carefully before putting the instrument into operation. The documentation contains information and warnings which have to be followed by the user in order to ensure safe operation of the instrument.

1.2.1 Symbols and conventions

The following symbols and styles are used in this documentation:

9	Numbers of the parts and controls see illustrations in <i>Section 2.2</i> .
	Instructions carry out the instructions step by step.
User	Parameters, input values Parameters and values for parameters, dialog title. Menu, menu item in the PC Control software.
[Next]	Button on the user interface. Fixed key on the Touch Control.
<Ctrl>	Key on the computer keyboard.
	Danger/Warning This symbol indicates a possible risk of injury to the user and possible damage to the instrument or its components.
	Attention This symbol indicates important information that you should read before continuing.
	Information This symbol indicates additional information and tips that may be particularly useful.

2 Installation

Connecting the Touch Control to the Titrande is described in the manual for the Titrande as well as the setup of the titration system with peripheral devices such as stirrers and dosing devices.

2.1 Setting up the Touch Control

2.1.1 Packaging

The Touch Control and its specially packed accessories are supplied in very protective special packaging. Please store this packaging in a safe place; it is the only way in which the safe transport of the instrument can be guaranteed.

2.1.2 Checks

Immediately after receipt, check whether the shipment has arrived complete and without damage by comparing it with the delivery note.

2.1.3 Location

The Touch Control has been designed for internal laboratory use and should not be used in explosion-endangered locations.

Place the instrument on a suitable vibration-free laboratory bench, protected as much as possible from corrosive atmospheres and contact with chemicals.

Choose a location where the temperature is usually between +5 °C and +40 °C. The instrument should be protected against excessive variations in temperature and direct sunlight.

2.2 Touch Control parts and controls

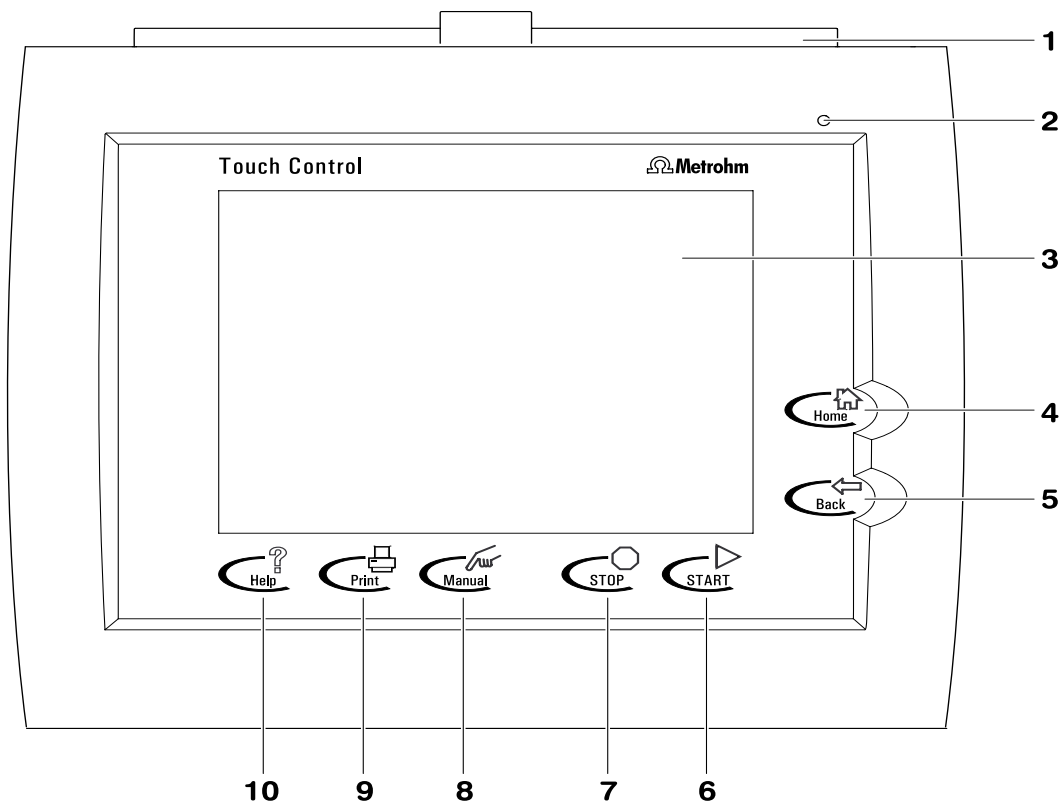


Fig. 2.1: Front view of the Touch Control

1 Protective cover for card slots

Accommodates two PCMCIA or CompactFlash memory cards.

2 “ON” LED

Lights up when instrument is switched on.

3 Touch Screen display

6 Fixed key [START]

Starts the current method.

7 Fixed key [STOP]

Stops the run.

8 Fixed key [Manual]

Opens the dialog for manual operation of the titration system.

4 Fixed key [Home]

Changes to main dialog.

9 Fixed key [Print]

Opens the print dialog for manual printout of a report.

5 Fixed key [Back]

Changes to previous dialog.

10 Fixed key [Help]

Opens the context-sensitive help.

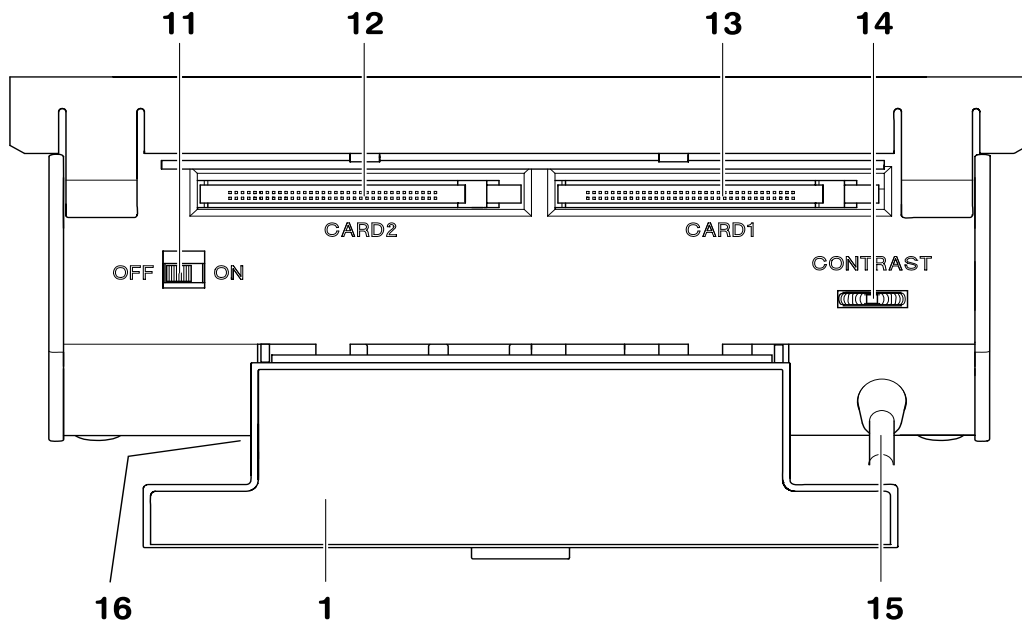


Fig. 2.2: Rear view of the Touch Control

<p>1 Protective cover for card slots Must be closed during operation to protect the electronics from splashes.</p>	<p>14 Contrast controller for display</p>
<p>11 On/Off switch Touch Control must be shut down properly by switching it off before the current supply is interrupted.</p>	<p>15 Connection cable for connecting the Touch Control to the Titrando ("Controller" connection).</p>
<p>12 Card slot 2 Accommodates one PCMCIA or CompactFlash memory card.</p>	<p>16 Type plate With device number and serial number</p>
<p>13 Card slot 1 Accommodates one PCMCIA or CompactFlash memory card.</p>	

3 Operation

The most important points concerning the operation of the Touch Control and PC Control are described in this section. As the appearance of the **operator interface** and the functions are almost identical, only the **PC Control** operator interface is shown. If individual functions are only available in **Touch Control** or in the PC Control software then this is indicated accordingly in the text.

The arrangement of the program and the **operating concept** are identical for Touch Control and the PC Control software. In **Touch Control** operation is carried out via a touch-sensitive screen (Touch Screen), in **PC Control** the software is operated by using a mouse and the PC keyboard. This results in several system-specific operating possibilities.

3.1 Operating principles: Touch Control

3.1.1 Switching Touch Control on and off

A Touch Control which is properly connected to a Titrande is switched on and off with ON/OFF switch **11** on the rear panel of the instrument.



Attention!

*The Touch Control must be **shut down properly by switching it off** with the ON/OFF switch on the rear panel of the instrument before the current supply is interrupted. Otherwise there is the risk that data may be lost. As power is provided to the Touch Control via the Titrande, the Titrande must never be separated from the mains supply (e. g. by switching it off via a multiple outlet strip) before the Touch Control has been switched off. When the Touch Control is **switched on** all the other peripheral devices (e. g. printer) must already be switched on.*

We recommend the following procedure:

- ☞ Connect all the instruments (Titrande and peripheral devices) to the mains supply via a **multiple outlet strip with mains switch**.
- ☞ When **switching on** first switch on the multiple outlet strip with the Touch Control switched off. Then switch on the Touch Control.
- ☞ When **switching off** proceed in the reverse order. First switch off the Touch Control. Then switch off all the peripheral devices via the multiple outlet strip switch.

3.1.2 Setting the display contrast of the Touch Control

Knob **14** for setting the contrast of the Touch screen is located on the rear panel of the instrument. Move it in one direction and hold it tight when it reaches the stop in order to increase or reduce the contrast.

- ☞ Use the fixed key **[Help]** in the main dialog to open the online help. Set the contrast so that the scroll bar surface is light gray and the margins to the left and below are dark gray (see Section 3.3.2).

3.1.3 Operating the Touch Screen

The whole screen surface is touch-sensitive. Just touch some of the buttons on the screen to see how to operate the Touch screen. You can always return to the main dialog by touching **[Home]**.

In order to **activate** an element on the Touch Control user interface just touch the screen with your fingertip, finger nail, the eraser of a pencil or a stylus (special tool for operating Touch screens); see below:

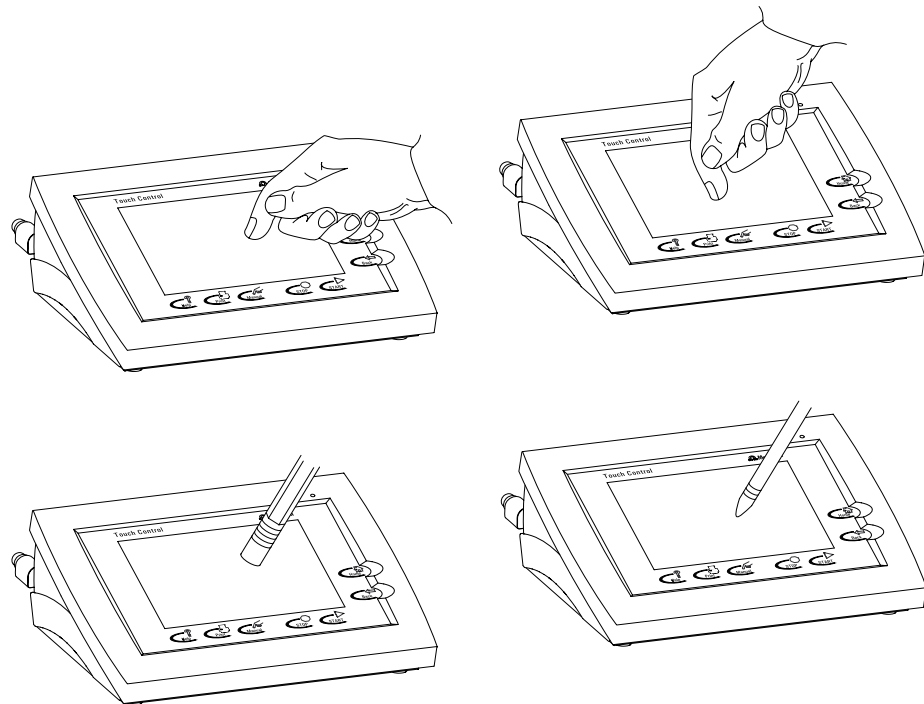


Fig. 3.1: Different ways of navigation on the Touch Screen



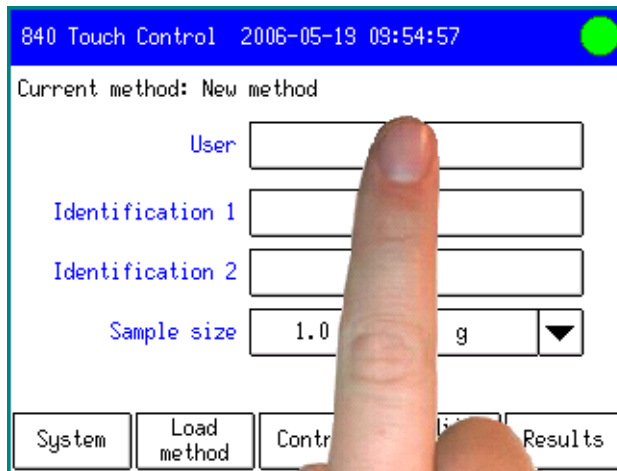
Attention!

Never touch the Touch screen with a pointed or sharp object such as a ballpoint pen.

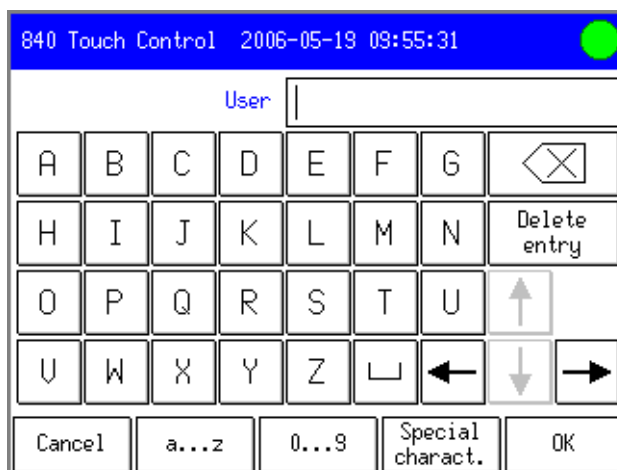
If you use the standard settings then touching an active operating element creates a sound.

3.1.4 Entering text and numbers using Touch Control

☞ Just touch an input field, e. g. **User** in the main dialog, to open the **Text editor**.



In the text editor the name of the parameter is shown in front of the input field.



☞ Touch the required character. Apart from the capital letters which first appear, there are also sets of characters with lower case letters, numbers and mathematical signs as well as three blocks of special characters. You can switch to the required set of characters with the **[a...z]**, **[0...9]** and **[Special characters]** buttons and between the blocks of special characters with **[More]**. The backspace button **[⊞]** deletes the character in front of the cursor. **[Delete entry]** deletes the whole text. With the arrow buttons the cursor can be positioned in the text.

☞ Accept your entry with **[OK]** or **[Back]**, or reject it with **[Cancel]**.

In input fields for numerical values the **number editor** will open. The required value is entered directly via the indicated keys. A stop is automatically used as the decimal separator.

☞ For example, touch the input field for the **Stop volume** in a titration command.

Edit command / Stop conditions			
Stop volume	100.000 mL		
Input: 0.00000 ... 9999.99	7	8	9
Default value: 100.000	4	5	6
	1	2	3
	0	+/-	.
			off
			R1 ▼
Cancel	Delete entry		OK

To the left of the block of numbers you can see the **input range** together with its **default value**. If not only numbers but also **special values** (e.g. **off**) can be entered for a parameter then the corresponding buttons will be shown to the right of the block of numbers. For many method parameters it is also possible to enter a result which has previously been defined in the method sequence as a value. The result variable can be selected under **[R1]** (see *Section 4.5.1*).

- ☞ Touch the required number or special value. The whole entry can be deleted with **[Delete entry]**.
- ☞ Accept your entry with **[OK]** or **[Back]**, or reject it with **[Cancel]**.

To make the entry of texts and numbers easier you can also connect an external PC keyboard with a USB connection to a Titrand system with Touch Control (see *Section 3.10.14*).

3.2 Operating principles: PC Control

3.2.1 Starting and stopping the PC Control software



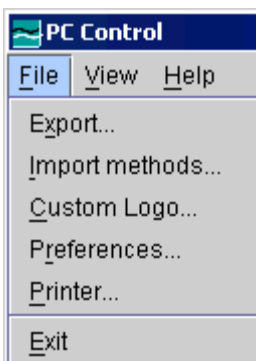
A double-click on the **PC Control icon**, which is automatically copied onto the Windows desktop during installation, starts the program. Alternatively you can start the program in the menu Start/Program Files/Metrohm/PC Control or execute the file PcControl.exe under C:\Program Files\Metrohm\PC Control\bin (installation with the default path) with a double-click. After the program start the main dialog window opens (see *Section 3.3*).



The program can be closed by either clicking on **[X]** (close) in the top right-hand corner of the program window or by clicking on the menu item **Exit** in the **File** menu. When the PC Control software is started the program window cannot be closed.

3.2.2 Operating the PC Control software

The **PC Control** program is operated within the main dialog window in exactly the same way as Touch Control. All the elements of this program window as well as the fixed keys can be activated or selected with a mouse-click.



PC Control also has a **menu bar** via which the specific PC Control functions can be selected.

In addition, the controls of the main dialog display can be accessed and operated via the **PC keyboard**. A cursor is provided; this can be moved from one item to the next by using the tab key. An item selected in this way is activated by the space bar. Input fields can be edited directly.

3.3 User interface and controls

3.3.1 User interface of the Touch Control and PC Control

In both cases the user interface consists of the **dialog window** itself and the **fixed keys**.

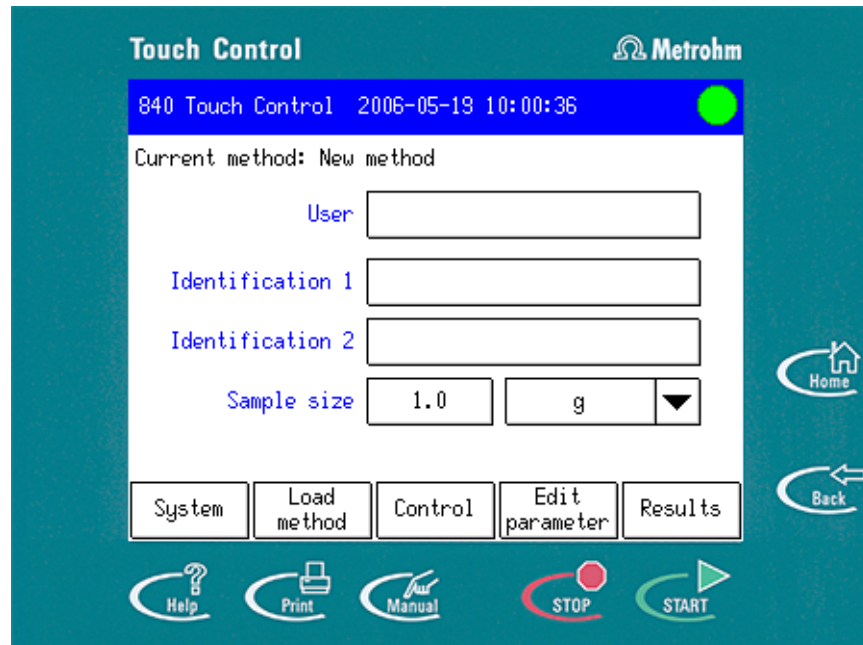


Fig. 3.2: Touch Control user interface

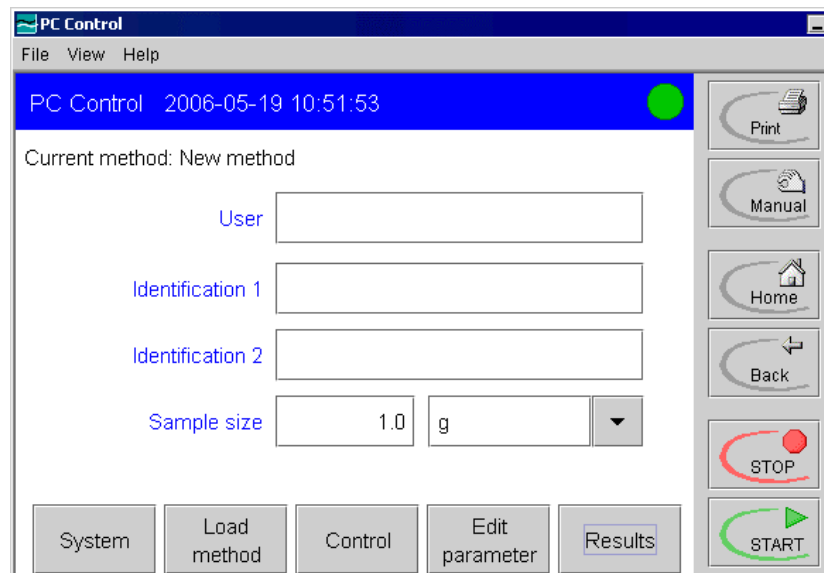

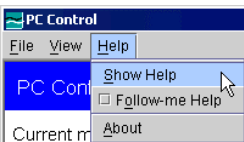











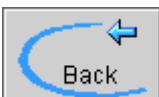


Fig. 3.3: PC Control user interface

The PC Control program has an additional **menu bar**.

3.3.2 Controls of the Touch Control and PC Control

Both the Touch Control and the PC Control software systems have changing controls within the dialog window and fixed keys outside the dialog window which are accessible at all times. The following table lists the functions of all the controls:

Fixed keys		
Touch Control	PC Control	Fixed key function
		Opens the context-sensitive online help function (see Section 3.3.3).
		Opens the print dialog for the manual printout of the reports (see Section 3.23).
		Opens the dialog for the manual operation of the titration system (see Section 3.24). With the PC Control a separate dialog window is opened.
		Stops the determination sequence. The command which is currently being processed will be stopped immediately and the results page will be shown (see Section 3.20.3). The following commands (e. g. calculations, REPORT commands) will not be carried out.
		Starts the current method; this will then be processed (see Section 3.20).
		Switches to main dialog.
		Switches to previous dialog.



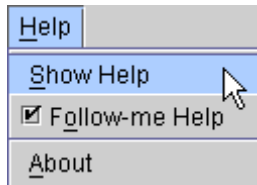
Note!

The settings made in a dialog window with **PC Control** will only be stored when the dialog is exited with **[Back]** or **[Home]**.

Dialog elements		
Touch Control	PC Control	Fixed key function
		Active buttons are indicated by a frame. Inactive buttons are shown in gray.
<input checked="" type="checkbox"/> Sample data silo	<input checked="" type="checkbox"/> Sample data silo	Tip or click on a checkbox to activate it.
		Use the scroll bar in order to navigate quickly through lists or longer text displays. To move up and down in the list push the scroll bar up and down with your finger or with the left-hand mouse key pressed down.
		The selection list can be recognized by the arrow to the right of the text. In an open list the element currently selected is shown with a background bar. Select the required element in the list with the finger or mouse. This entry will then be transferred directly to the input field.
		If the input field and arrow are separated by a line then this means that you can also make your own entries. In the Touch Control you can open the text editor by touching the input field. In PC Control you can click directly on the input field and enter text/numbers. The selection list is opened with the arrow.
		In the list the selected line is indicated by a light blue bar. You should first mark the line to be selected and then activate the button for the function you want to apply to the selected element.

3.3.3 Online help

This manual is chiefly intended to describe the procedure for configuring the system, carrying out a determination and evaluating and storing the data. For further details about the individual parameters, e. g. input ranges, you should use the context-sensitive online help, which will rapidly provide you with the information you require at any point.



In **Touch Control** you can open the online help with the **[Help]** fixed key. In the **PC Control** software the online help is opened with the <F1> key on the computer keyboard or started by clicking on the menu item **Show help** in the **Help** menu. If you also activate the item **Follow-me help** in this menu then the help window will be updated each time that the dialog is changed.

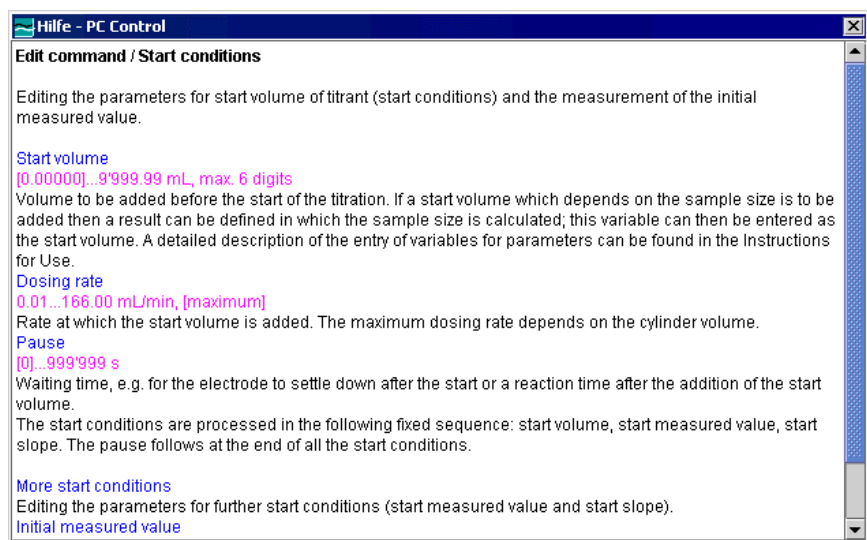


Fig. 3.4: Online help, PC Control

The following markings apply to the online help for Touch Control and PC Control:

- Blue text** Parameters and buttons which are explained.
- Violet text** Input values for the parameters.
- [Value]** Default value for a parameter.

3.4 Program structure

The program structure is arranged so that the most important functions can be accessed with only a few clicks **or touches on the** buttons. Functions which are not often used in routine operation, such as changing the system settings or editing individual parameters in a method, can be found in lower dialog levels. In order to provide an overview of the structure of the program we have summarized the most important functions in the following diagram:

Main dialog

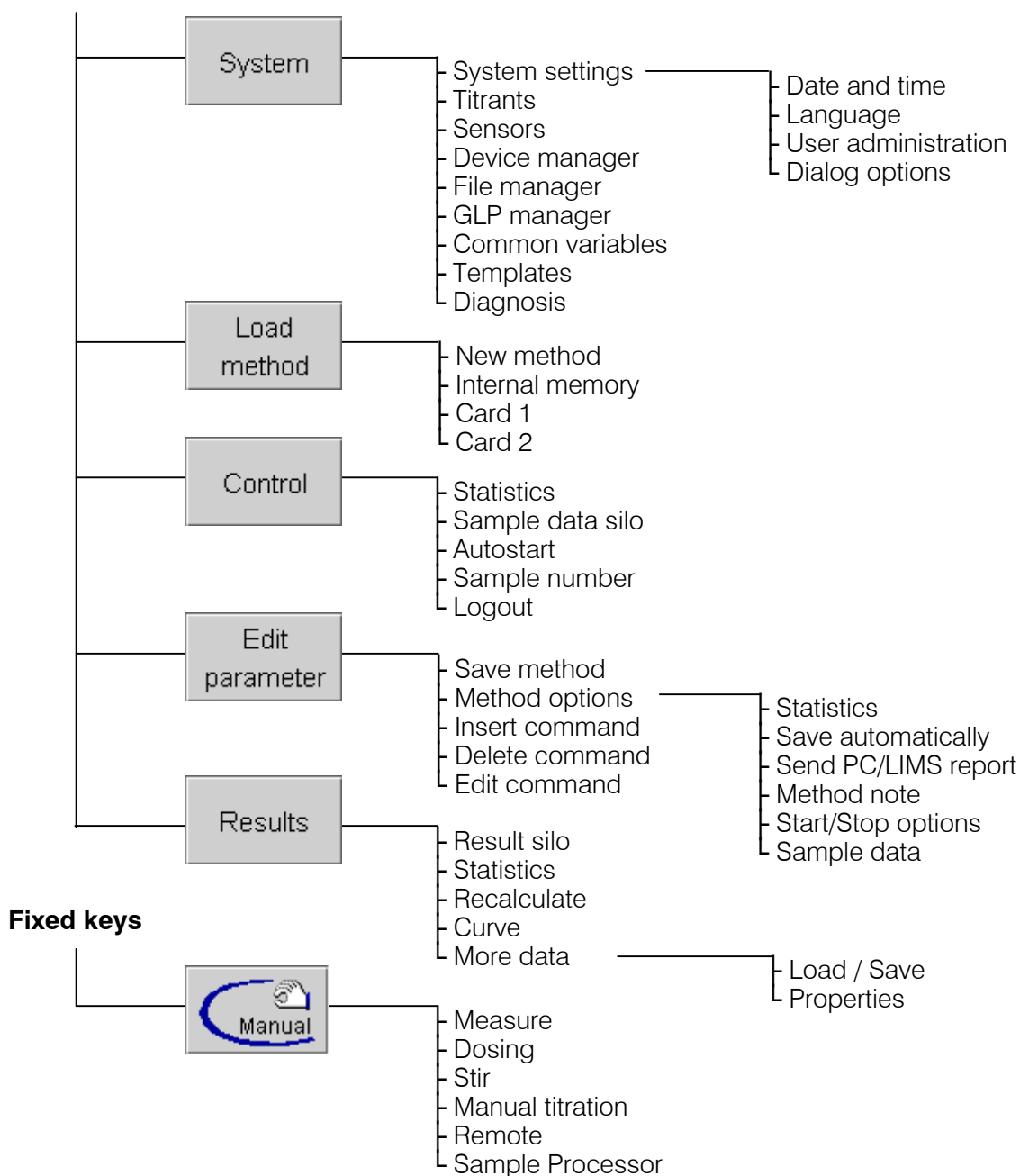
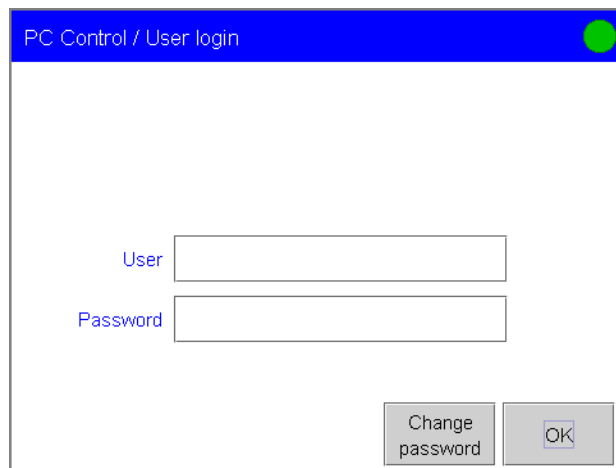


Fig. 3.5: Program structure

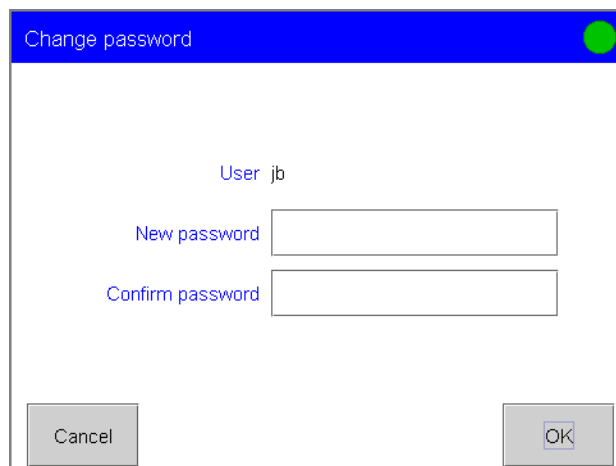
3.5 Login

Depending on how your Titrand system is configured, you may have to use the **User login** function before you can work with the system. User administration is carried out by a user with administrator rights (see *Section 3.7.5* to *Section 3.7.7*). There are two different ways of identifying the user: by the **entry of the user name** or by using an **identification card**, on which the user name and the routine dialog settings are stored. If a **password** is required for identification then this will be requested on login in both cases.

In the following example the user must identify himself/herself by entering a name and password.

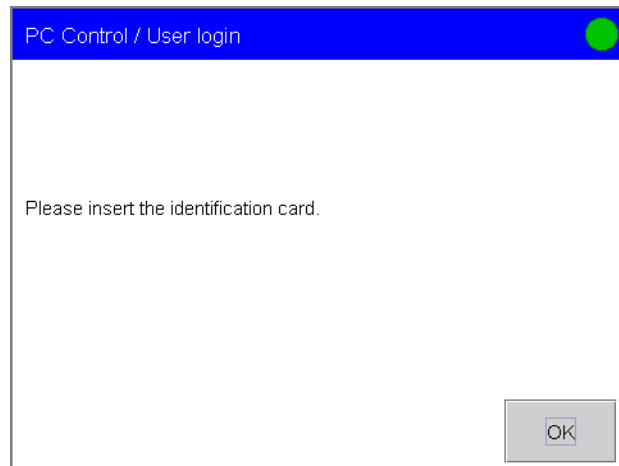


The first time that you log in you must first define your password with **[Change password]**:



- ☞ First enter the password under **New password** and enter it again under **Confirm password** for confirmation. Please note that this password can not be used multiple times.
- ☞ Enter your **password** in the login dialog. If the user is defined in the list of users and if the correct password has been entered then the main dialog will open.

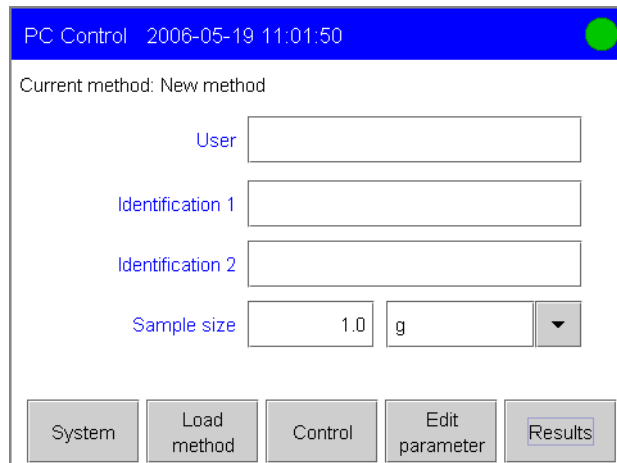
If you have to identify yourself with an identification card then you will be requested to insert it.









In **Touch Control** you must always insert your identification card in Card slot 1. In **PC Control** ask your system administrator to tell you the drive to be used. If a password additionally has to be entered then the corresponding dialog will be opened automatically; otherwise the main dialog will open directly.



3.6 Main dialog and structure of the dialog windows

This section provides an overview of the structure of the dialog windows and the various dialog elements. The user interface without the fixed keys **[Help]**, **[Print]**, **[Manual]**, **[STOP]**, **[START]**, **[Home]** and **[Back]** is known as the **dialog window** (or just dialog):

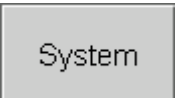


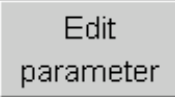



- In the **status line** (blue bar) the titles of the previous dialog and current dialog are normally shown. Only in the main dialog the type of instrument and the actual date and time are shown in this status line. In the live display (see Section 3.20.4) the name of the current method is shown.
- In the right top corner the current **status** of the system is shown:

	Instrument in normal working condition (ready), i.e. a determination can be started.
	Conditioning is running (for SET and KFT titrations)
	Conditioning has been manually stopped with [Hold] . It can be continued with [Continue] .
	Conditioning is finished; the sample will be titrated up to the endpoint and held there.
	A determination sequence has been started. [START] and [Print] are not active now.
	The determination sequence has been interrupted manually with [Hold] or automatically. It can be restarted with [Continue] .

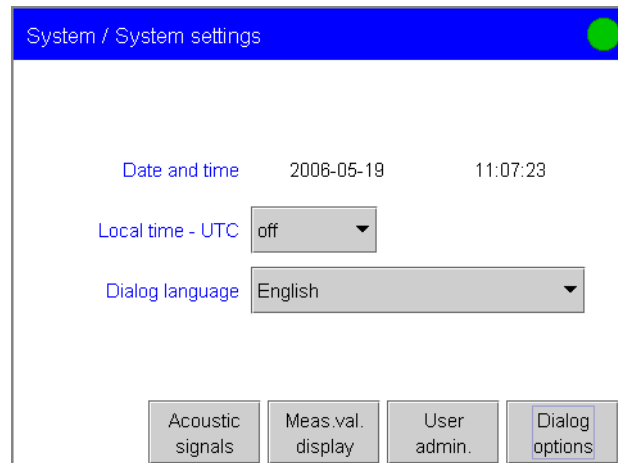
	<p>A run has been started in the "Manual control" dialog window.</p>
	<p>A fault has occurred during the manual operation of the System.</p>

- In the **main dialog** you can enter or select the **user** if you are not working with login (see *Section 3.7.5*). You can also edit the **sample data** (see *Section 3.19.1*).
- The buttons at the lower margin of the dialog change their function according to the dialog shown. They are usually used to open a new dialog. You can open the following dialogs from the **main dialog**:

	<p>Instrument-specific system settings, titrant and sensor management, management and configuration of peripheral devices, file management, GLP functions, edits system-specific variables, creates various templates, diagnostic functions and software updates.</p>
	<p>Loads a method from the method memory and creates a new method.</p>
	<p>Switches statistics on/off, switches sample data silo on/off, deletes sample data silo (Touch Control only), autostart, sample number, system logout and deletes statistics.</p>
	<p>Edits method command list and the parameters of the current method.</p>
	<p>Shows the results of the current determination, recalculation and re-evaluation of the current determination, views, saves and loads determination data, views statistics results and results silo.</p>

3.7 System settings

A range of system-specific settings and configurations is described in this section. You should first select the dialog language and set the date and time. You can also configure the dialog for routine use and create a list of users. You can make various settings concerning the measured value display and output of acoustic signals.



3.7.1 Selecting the dialog language

- ☞ Open the dialog **System/System settings**.
- ☞ Open the selection list **Dialog language** with the arrow and select the language.
- ☞ Exit the dialog with **[Home]** so that the setting applies to all dialogs. (From this particular dialog you can also return to the main dialog with **[Back]**.)

3.7.2 Setting the date, time and time zone

PC Control and **Touch Control** show date and time according to ISO standard 8601.

- ☞ Open the dialog **System/System settings**.

With **PC Control** the date and time will be taken directly from the operating system of your computer. The change from Summer to Winter time and vice versa is made automatically.



Note!

In order for the **summer / winter time** to be taken into account in the **Windows time display** you must activate the checkbox **Automatically adjust clock for daylight saving changes** under **System settings** in the menu **Date/Time Properties** under **Time Zone**.

With **Touch Control** you should set the date and time as follows:

- ☞ Open the date editor by touching the input field for the **date**.
- ☞ Enter the actual date in the format year (4-place)-month-day. The hyphens are already present. Confirm the entry with **[OK]**.

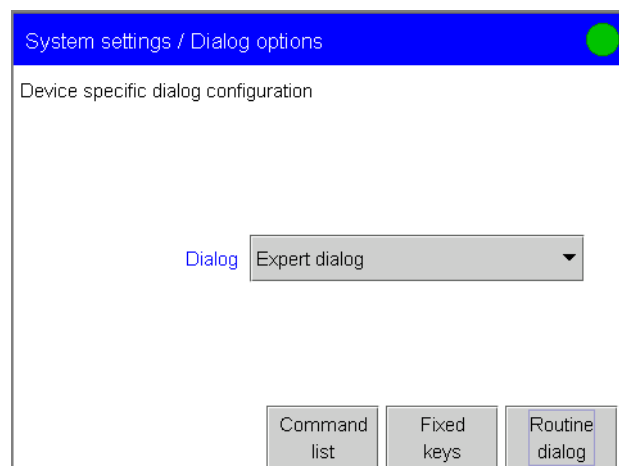
- ☞ Open the editor for the **time** by touching the input field for the time.
- ☞ Enter the actual time in the format hours:minutes:seconds. The entry should be made in the 24-hour format. The colons already exist. Confirm the entry with **[OK]**.

By entering a **local time** the time information becomes unambiguous. You can enter the local time for both PC Control and Touch Control. It is printed out in the report header together with the date and time. With PC Control the difference to UTC (Coordinated Universal Time) is taken automatically from the system settings of the PC.

- ☞ In the **local time** input field you should enter the time zone based on UTC (Universal Time) or switch off the function (example: – 05:00).

3.7.3 System-specific dialog options

The functions which a user can access can be configured specifically for the system. You can define which method commands and fixed keys can be used, and whether the system is to be operated in expert dialog (all functions accessible) or in routine dialog (individual functions disabled). The buttons to be disabled in routine dialog can also be system-specifically defined. If an identification card is provided for each user (see *Section 3.7.6*) then the routine dialog settings can also be stored user-specifically on the card.



If you are not working with login then you can system-specifically choose whether the system is to be operated in **expert dialog** or **routine dialog**. In expert dialog all functions are accessible. In routine dialog you can disable individual functions under **Dialog options /Routine dialog**.

- ☞ Select either **Routine dialog** or **Expert dialog** under **Dialog** in **System settings/Dialog options**.
- ☞ Exit the dialog with **[Home]** so that the setting applies to all dialogs.



Note!

If you have selected **Routine dialog** and the dialog **System settings/Dialog options** is disabled for routine dialog then you can change back to expert dialog by entering **Metrohm** as the user in the main dialog. If you are using login then a user who works with expert dialog must log in.

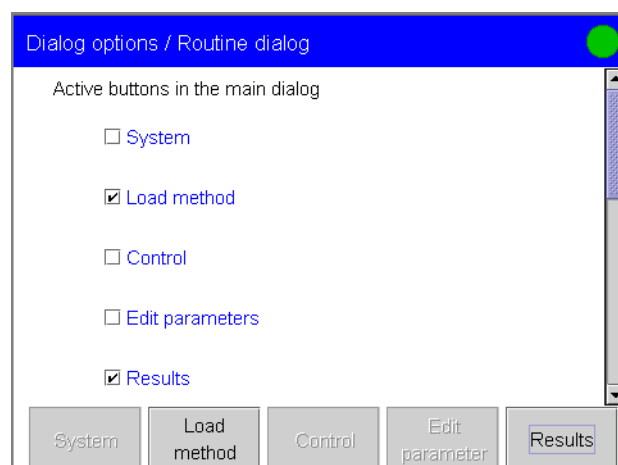
The selection of **method commands** (list of commands) and the **fixed keys** (**[Print]** and **[Manual]** only) which can be used can only be opened when the system is being operated in expert dialog.

- ☞ Open the **Dialog options/Command list** dialog.
- ☞ Disable the checkboxes for the command groups which are not to be used. These will then be shown in gray in the method editor for the selection of the commands. These settings apply to both expert dialog and routine dialog.
- ☞ Open the **Dialog options/Fixed keys** dialog. Only the **[Print]** and **[Manual]** (manual operating of the titration system) fixed keys can be disabled.
- ☞ Disable the checkboxes for the fixed keys which are not to be used. These settings apply to both expert dialog and routine dialog.

3.7.4 Routine dialog: disabling functions

A standard configuration which is suitable for routine dialog is stored: methods can be loaded but not altered or newly created. Determination data (results) can be viewed and saved, but not modified. You can adapt this standard configuration as follows:

- ☞ Open **Dialog options/Routine dialog** in order to deactivate those buttons which are to be disabled in the main dialog, the live display and in manual control. With PC Control you can also disable individual menus. This dialog can only be opened when the system is being used in expert dialog.



- ☞ Deactivate the checkboxes for the functions which are to be disabled in routine dialog.

You can disable individual functions in the corresponding dialogs with the buttons at the lower margin of the dialog window (**[System]**, **[Load**

method], **[Control]**, **[Edit parameter]** and **[Results]**). In order for the button to be active the corresponding checkbox must be activated above.

☞ Open the dialog in which you wish to **disable buttons** and deactivate the checkboxes for the buttons that are to be disabled for routine dialog.

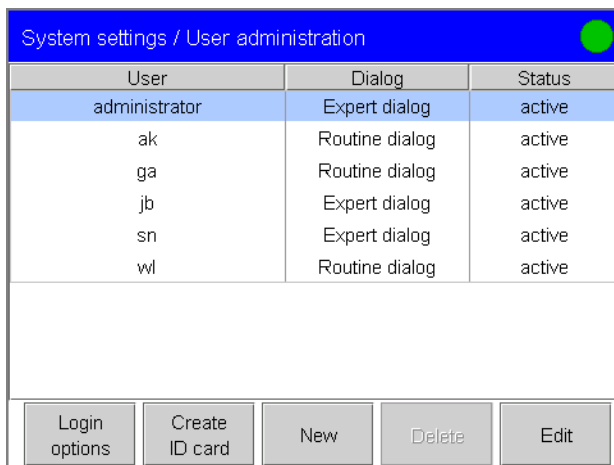
You can also disable buttons in several subdialogs. These are indented so that you can see which buttons belong to which dialog.

3.7.5 User administration

You can draw up a system-specific **list of users** who can operate the titration system. You can use this list in two different ways: if you work with **login**, i.e. if each user must log into the system before starting work, then only those users entered in the list can log in. The user who is currently logged in is shown in the main dialog and cannot be edited. If you work without login then in the main dialog you can select the user from those entered in the list and document the user of the titration system in this way. The user name is printed out in all reports containing determination data and stored in the determination file. Each file always contains the name of the user who created it and the name of the last user to edit it.

The name of the user, the dialog that the user can use to operate the system and the status of the user are shown in the **user list**. If you work with login then this dialog is only accessible to users with administrator rights.

☞ Open the dialog **System settings/User administration**.



User	Dialog	Status
administrator	Expert dialog	active
ak	Routine dialog	active
ga	Routine dialog	active
jb	Expert dialog	active
sn	Expert dialog	active
wl	Routine dialog	active

Buttons: Login options, Create ID card, New, Delete, Edit

The user list is initially empty.

☞ Use **[New]** to define all the users who are allowed to operate the system.

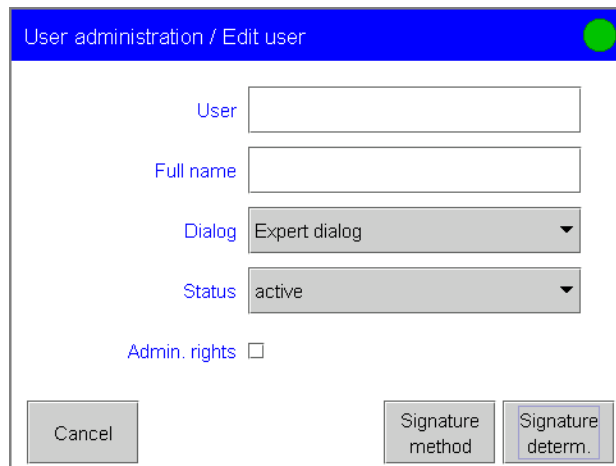
The dialog in which the **user data** can be entered is opened automatically with **[New]**. For an existing user this dialog can be opened with **[Edit]**. Existing users can be removed from the list with **[Delete]**.



Note!

If you once have worked with login and password protection then it is no longer possible to delete users from the list even if the password protection is switched off again.

The list of users can only be printed out in a context-sensitive situation from the dialog **System settings/User administration** and its subdialogs by using the **[Print]** fixed key. This means that only users with administrator rights can print out this list.



- ☞ Enter an unambiguous identification under **User**, for example the in-house abbreviated form of the name or the personnel number. Each user name can only appear once in the list of users.
- ☞ Under **Full name** enter the proper name of the user, i.e. given name and family name.
- ☞ Select the **Dialog** in which the user is to operate the system.

This setting is only effective when login is used. In **Expert dialog** all functions are accessible. For **Routine dialog** the system-specific routine dialog configuration is normally used (see Section 3.7.3). If each user is to have separately defined routine dialog settings then you can create an identification card for each user on which these settings are stored (see Section 3.7.6). During login the dialog settings stored on the card will be loaded automatically.

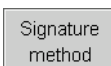
The **user status** normally remains **active**. It is a good idea to deactivate a user when, for example, he or she is absent for a long time or is no longer authorized to use the system. This user can then no longer log into the system until the **active** status is reactivated.

- ☞ You should activate the **Administrator rights** checkbox for each user who is to have access to the user administration.



Note!

The last user with administrator rights cannot be deleted.



By clicking on **[Signature method]** you can access the edit dialog for assigning the rights for using and signing methods. These settings are only effective when login and password is used. Only methods with the

status **"Saved"** can be signed. The status of the method is given under **Method options/Properties** (see Section 3.16.9).



Edit user / Signature method

- Use only released methods
- Review methods (signature level 1)
- Release methods (signature level 2)
- Delete signatures

If **use only released methods** is activated then the corresponding user can only use methods that have been released, i.e. can only start methods that have been signed at level 2. **Review methods (signature level 1)** must be activated for a user to be entitled to sign a method at level 1. The method then receives the status "Reviewed". To be able to sign methods at level 2 **Release methods (signature level 2)** must be activated. A method can only be signed at level 2 when it has already been signed at level 1. The same user can sign different methods either at level 1 or at level 2, if both checkboxes **Review methods** and **Release Methods** are activated but not the same method at the same time at level 1 and at level 2. When the user has signed the method at level 2 it receives the status "Released". If **Delete signatures** has been activated for a user then the user is entitled to delete signatures. However, this is possible for methods that have been signed at level 2. All the signatures are deleted and the method receives the status "Saved".

The methods can be signed under **Method options/Properties**. The procedure is described in Section 3.16.3.

Signature
determ.

By clicking on **[Signature determination]** you can access the edit dialog for assigning the rights for using and signing determinations. These settings are only effective when login and password is used.



Edit user / Signature determination

- Review determinat. (signature level 1)
- Release determinat. (signature level 2)
- Delete signatures

In a similar way to that used for methods, it is possible to state whether a user is entitled to sign determinations at level 1, i.e. to **Review determinations**, and/or is entitled to **Release determinations**, i.e. to sign them at level 2. If **Delete signatures** has been activated for a user then the user is entitled to delete signatures. As in the case of methods, this is only possible when a determination has already been signed at level 2.

Determinations can be signed under **More determination data/Properties**. The procedure is described in Section 3.18.4.


Attention!

*If you work with **Login** then **User administration** is only accessible to users with administrator rights. This means that you must ensure that at least two users have administrator rights so that one of them is almost always available. Keep the rights of access for a user with administrator rights in a safe place so that it is accessible in an emergency.*

3.7.6 Creating an identification card

If you have selected the version **Login via identification card** under **User administration/Login options** (see Section 3.7.7) then you must provide each user with an identification card. The identification card has the **User name** and the current **routine dialog settings** stored on it (see Section 3.7.4).

During login with an identification card a check is made that the user is present in the list of users and whether expert dialog or routine dialog is to be used. After a successful login the routine dialog settings stored on the card are loaded into the system. These define the buttons and functions that are accessible to the user if routine dialog is used.

If you wish to provide separate routine dialog settings for each user then you must always adapt these settings (see Section 3.7.4) before you create the identification card for the particular user. These **user-specific routine dialog settings** are stored on the identification card with the name of the user.

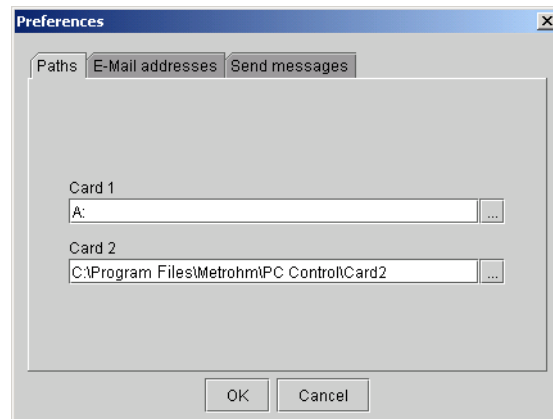
Touch Control

With Touch Control the identification card is always created in **Card slot 1 (13)**, see Fig. 2.2: *Rear view of the Touch Control*).

- ☞ Insert the data card into Card slot 1.
- ☞ In the user list, select the user for whom you would like to create the identification card.
- ☞ Press **[Create ID card]**. The settings are stored.

PC Control

- ☞ Open the menu **File/Preferences**.
- ☞ Define the drive in which the identification card is to be used under **Paths** for **Card 1** (see Section 3.11).



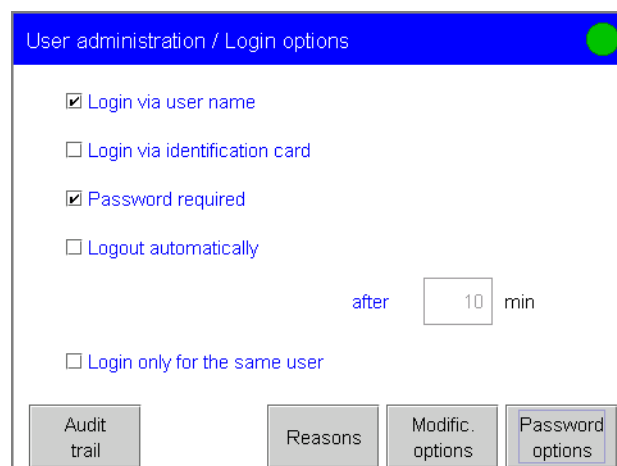
Select the disk drive if you want to use diskettes as identification cards. You can also use a card drive with PCMCIA FlashCards or CompactFlash cards, or a USB memory stick. With external drives you must always check how to recognize when a storage process has been completed in the user manual for the drive. This is usually indicated by an LED. If you use the PCMCIA card drive of a laptop computer then you should always trigger "Remove hardware" in the operating system before removing a card from the drive. This is the only way that you can be sure that the data has been stored when you remove the card.

- ☞ In the user list, select the user for whom you would like to create the identification card.
- ☞ Press [**Create ID card**]. The settings are stored.

3.7.7 Editing login options

There are various ways of logging in to the system: either the user name is requested or identification is carried out by using an identification card (see *Section 3.7.6*). It is also possible to combine both versions.

- ☞ Open the dialog **User administration/Login options**.



- ☞ Activate the checkbox(es) for the **login option(s)** that you wish to use.



Attention!

If you select **Login via identification card** then you must create an identification card for each user.

Once you have selected a login option you can then make further settings for logging in:

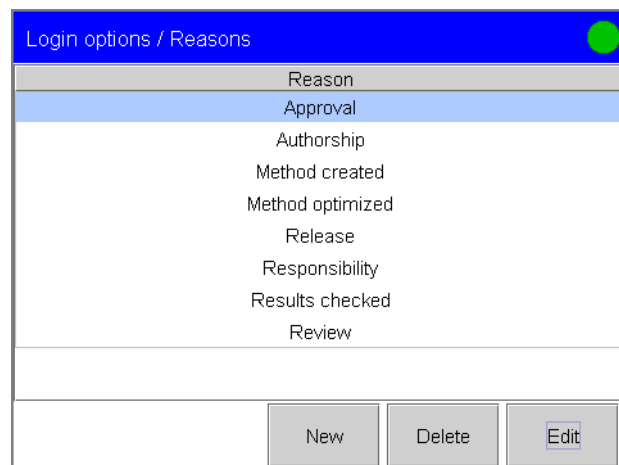
- ☞ If a password is to be requested as well as the user name then you must activate the **Password required** checkbox. If this function is switched on then it is no longer possible to delete users from the list of users; they can only be deactivated. This is a requirement for complying with **FDA Guideline 21 CFR Part 11**. The various settings for entering a password are carried out under **[Password options]** (see p. 32).
- ☞ Activate the **Logout automatically** checkbox if the user is to be logged out of the system automatically after a certain time has elapsed. Enter the interval after which the logout is to take place automatically.



Note!

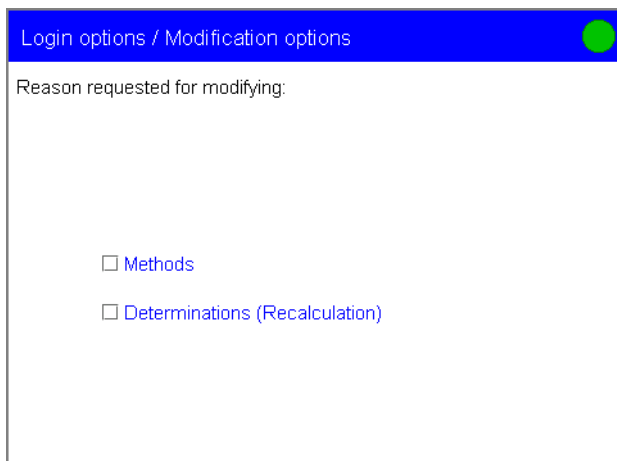
When you exit this dialog (**User administration/Login options**) with **[Back]** or **[Home]** after you have activated one of the login options **Login via user name** or **Login via identification card** then you will automatically find yourself in the login dialog and will have to log into the system. This means that you must make sure that you have first defined all the users and produced the identification cards before you activate login.

Under **[Reasons]** you can draw up a selection list containing reasons from which a selection can be made when signing and modifying methods and determinations. Some reasons have already been provided.



- ☞ You can insert a new reason in the list with **[New]**. Existing reasons can be deleted from the list with **[Delete]** and existing reasons can be renamed with **[Edit]**.

Under **[Modification options]** you can select in which cases a reason is to be demanded.



Login options / Modification options

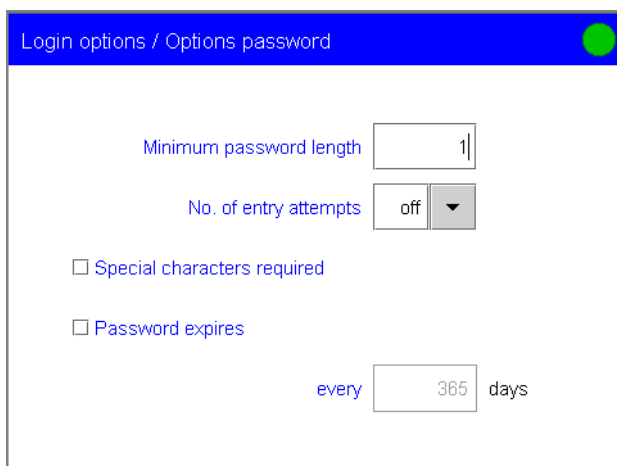
Reason requested for modifying:

Methods

Determinations (Recalculation)

If you activate **Methods** then when a modified method is being saved a reason for the modification will be demanded. Results are altered when a determination is recalculated. If you require a reason to be given in such cases then activate the **Determinations** checkbox. The reasons are only demanded when login and password is used.

These reasons are documented in the audit trail (see *Section 3.7.8*) together with the alteration. The reason for the last modification is shown in the properties of the method or determination.



Login options / Options password

Minimum password length

No. of entry attempts

Special characters required

Password expires

every days

☞ You should now edit the password options. You can define a **minimum length** for the passwords to be used. This will be checked when a user enters a new password. After the maximum **Number of entry attempts** during login the user will be automatically deactivated and can only be reactivated by a user with administrator rights. The use of certain **Special characters** in the password can be demanded (see **online help**). You can also define a time limit after which the password must be altered. Changing a password, it is not possible to choose one which was already used before.

In the **Titrand Compliance Guide** there is a step by step description of the necessary procedure for complying with **FDA Guideline 21 CFR Part 11**.

**Attention!**

If a user has forgotten his password, a new user name has to be defined. The same user name can only be used again after a new installation and the recreating of the user list. Proceed therefore as follows:

PC Control:

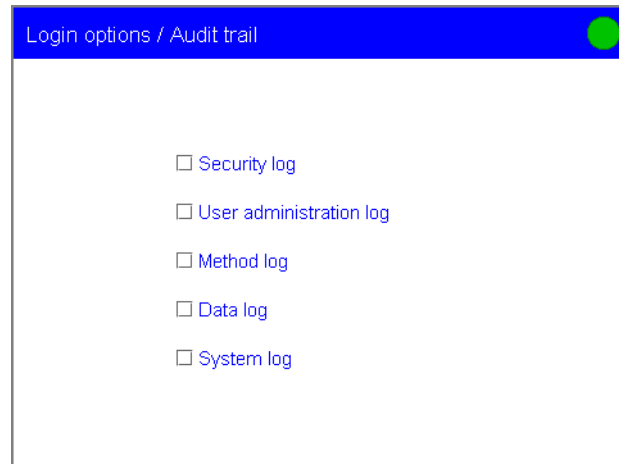
- ☞ Carry out a backup (see *Section 3.11.6*).
- ☞ If you have defined the PC Control installation directory as location for the backup (under File/Preferences/Paths), copy the **folder "Backup"** to another position.
- ☞ Uninstall the PC Control software. In order to uninstall the software completely, all the folders in the installation directory must be deleted.
- ☞ Install the PC Control software again.
- ☞ Move the folder "Backup" to its original position if necessary.
- ☞ Load the data from the backup into your system by using the function **Restore** (see *Section 3.11.6*). Deactivate the options **User list** and **System settings/User administration**.
- ☞ Create the user list again and define the login options.

Touch Control:

- ☞ Carry out a backup (see *Section 3.11.6*).
- ☞ Switch off the Touch Control and carry out a RAM initialization (see *Section 5.3.2*).
- ☞ Load the data from the backup into your system by using the function **Restore** (see *Section 3.11.6*). Deactivate the options **User list** and **System settings/User administration**.
- ☞ Switch off the Touch Control and switch it on again after a few seconds.
- ☞ Create the user list again and define the login options.

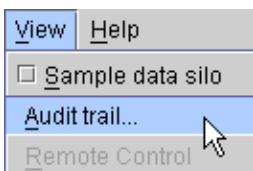
3.7.8 Audit trail

In the **Audit trail** all user actions are recorded together with the user name, date and time. Recording an audit trail is important for using PC programs to meet the requirements of **FDA Guideline 21 CFR Part 11**



☞ Under **System/System settings/User administration** in the dialog **Login options/Audit trail** activate the checkboxes for the data to be logged in the audit trail. The actions which should be logged can be found in the **online help**. In order to meet the requirements of **FDA Guideline 21 CFR Part 11** for an audit trail you must activate all the options.

You can also use the audit trail function specifically to record the data which interest you.



To view the recorded data in PC Control you should open the menu item **Audit trail** in the **View** menu.


No	Date	User	Category	Action	Details
1	2006-05-19 11:26:24		Admin	Change audit t. opt.	Security log off --> on
2	2006-05-19 11:26:24		Admin	Change audit t. opt.	User administration log off --> on
3	2006-05-19 11:26:24		Admin	Change audit t. opt.	Method log off --> on
4	2006-05-19 11:26:24		Admin	Change audit t. opt.	Data log off --> on
5	2006-05-19 11:26:24		Admin	Change audit t. opt.	System log off --> on
6	2006-05-19 11:26:58		Admin	Edit user	jb Jürg Expert dialog Status active Admin. rights on Use of
7	2006-05-19 11:27:02		Admin	Edit user	jb Jürg Expert dialog Status active Admin. rights on Use of
8	2006-05-19 11:27:40		Admin	Change sign options	jb Review methods (signature level 1) off --> on
9	2006-05-19 11:27:40		Admin	Change sign options	jb Release methods (signature level 2) off --> on
10	2006-05-19 11:27:40		Admin	Change sign options	jb Delete signatures off --> on
11	2006-05-19 11:28:18		Admin	Edit user	ak Angelika Routine dialog Status active Admin. rights off
12	2006-05-19 11:28:30		Admin	Change login options	Login via user name off --> on
13	2006-05-19 11:28:30		Admin	Change login options	Password required off --> on
14	2006-05-19 11:28:36		Admin	Change password opt.	Password expires off --> on
15	2006-05-19 11:28:36		Admin	Change password opt.	Password expires 365 --> 30
16	2006-05-19 11:28:48		System	Message	002-113 Method not saved Yes/OK
17	2006-05-19 11:28:48		Security	Logout	
18	2006-05-19 11:29:06	Admin	Security	Change password	
19	2006-05-19 11:29:10	Admin	Security	Login	Admin
20	2006-05-19 11:29:29	Admin	Method	New	Empty method
21	2006-05-19 11:29:38	Admin	Method	Insert command	New method V0 01 CAL pH
22	2006-05-19 11:29:44	Admin	Method	Edit	New method V0 01 CAL pH Stirrer off
23	2006-05-19 11:30:09	Admin	Method	Start	New method V0 1.0 g
24	2006-05-19 11:30:09	Admin	Method	Start	Start key pressed
25	2006-05-19 11:30:36	Admin	Method	Stop	New method V0
26	2006-05-19 11:31:14	Admin	System	Message	002-113 Method not saved Yes/OK
27	2006-05-19 11:31:14	Admin	Security	Logout	Admin
28	2006-05-19 11:31:28	jb	Security	Login message	Password expired
29	2006-05-19 11:31:40	Admin	System	Message	002-110 Password expired Yes/OK
30	2006-05-19 11:31:44	jb	Security	Change password	
31	2006-05-19 11:31:46	jb	Security	Login	Jürg
32	2006-05-19 11:32:11	jb	Method	New	Empty method
33	2006-05-19 11:32:36	jb	Method	Insert command	New method V0 01 DET pH
34	2006-05-19 11:33:08	jb	System	Message	010-003-1-X Other devices at MSB Yes/OK

Fig. 3.6: Audit Trail





The first column shows the **number of the entry**. The second column shows a **symbol** which classifies the entry: for information about actions which are neither security-relevant nor alter the determination data; for actions such as logging in and out of the system, changes to the login options and alterations to the determination data such as recalculations; for errors which may occur such as entering an incorrect password during login. The third column shows the **date**; the fourth column gives the **user** who carried out the action. The fifth column shows the **category** to which the entry belongs. The categories for which actions should be entered in the audit trail can be defined under **Login options/Audit trail** (see p. 34). The sixth and seventh columns show the **action** and **details** of the action. For alterations to a method the method name and version (e. g. V1) are always shown under details. V0 is shown for new methods which have not yet been saved. Behind this the number and name of the command are shown. The old value and new value, separated by an arrow, are always shown for alterations to variables or parameters.


Only users with administrator rights can export the audit trail as a text file. This means that the audit trail can be archived and made available for inspection whenever necessary. This is done by opening the menu

item **Export** in the **File** menu and entering the path and file name with the extension **.txt**. When the audit trail is exported its contents will be deleted. The audit trail window is closed with **Close**.

To **print** the audit trail click on the symbol  in the symbol bar or choose the report "Audit trail" in the dialog **Print/More Reports/System reports**.

Quick filters can be used on the audit trail entries:

-  Click on a cell in the table which meets the filter criterion.
-  In the **Filter** menu click on **Quick filter** or on  in the symbol bar. You can use the quick filter in succession for various entries.
-  To show all the entries again click on **Show all** in the **Filter** menu or on  in the symbol bar.


You can update the list with  so that new entries are also shown. The audit trail window is not automatically updated "live". When the audit trail window is opened the table is updated automatically.

You can view an external Audit trail i.e. from a Touch Control as well. Therefore load the desired Audit trail file in the Audit trail window under **File/Open**. With Touch Control the Audit trail file "**log.madt**" is created on the memory card in card slot 2. The entire path with file name is displayed in the title bar of the Audit trail window. An external Audit trail cannot be deleted in contrast to the internal Audit trail but the other functions remain the same.

To show the Audit trail of the running PC Control you have to close the audit trail window and open it again via **View/Audit trail**.





Note!

An external Audit trail can only be printed with the print symbol . When printing via the fixed key **[Print]** the internal Audit trail will be printed every time even if the external Audit trail is currently displayed.

In the **Titrand Compliance Guide** there is a step by step description of the necessary procedure for complying with **FDA Guideline 21 CFR Part 11**.

3.7.9 Measured value display

This setting refers only to the display of the measured values in the determination sequence (live display) and in manual operation (Manual Control). The values are always stored with their full resolution.

-  Open the dialog **System settings/Measured value display**.
-  Select **Number of decimal places** with which pH values and potentials are to be shown in the measured value display.

3.7.10 Acoustic signals

☞ Open the dialog **System settings/Acoustic signals**.

- **Show a message**: each time that a message appears on the screen a short beep will be heard. This informs the user that the message must be confirmed. This function is switched off by deactivating the checkbox.
- **Button contact** (Touch Control only): each time that a button is touched on the Touch Screen this will be confirmed by a beep. If you touch an inactive area of the Touch Screen then no beep will be heard.

☞ Exit the dialog with **[Home]** in order to accept the settings.

If you touch or click on a fixed key which should not be used at the moment (e. g. **[START]** when a determination is running) a beep will be heard to indicate an error.

3.8 Titrants

This section describes how you can draw up a list of titrants used in the system. These titrants can be used in intelligent type dosing units or intelligent type exchange units or in so-called non-intelligent exchange and dosing units. **Intelligent exchange and dosing units** have a built-in data chip on which **data about the reagent and the unit** can be stored. When the exchange or dosing unit is attached this data is read out automatically by the control device (Titrande, USB Sample Processor etc.) and entered in the **list of titrants**. You can also store the titrant data for reagents which are used in non-intelligent exchange or dosing units in the list of titrants.

The following **reagent data** is stored in the list of titrants:

- Titrant name
- Concentration with unit
- Comment
- Titer with unit
- Statistical information about last titer determination
- Period of validity for titer (with date for next titer determination)
- History of the last 10 titers
- Working life (with preparation date and expiry date)

The following **exchange or dosing unit data** is also stored:

- Designation (name)
- Order number (is read out automatically in case of intelligent exchange or dosing units)
- Serial number (is read out automatically in case of intelligent exchange or dosing units)
- Cylinder volume (is read out automatically in case of intelligent exchange or dosing units)
- Serial number of the cylinder (is read out automatically in case of intelligent exchange or dosing units; however, must be re-entered if the cylinder is changed)
- Length and diameter of the tubing and port occupancy of the dosing unit
- Parameters for preparing the exchange or dosing unit
- Direction of rotation of the valve disk (dosing unit only)
- Time interval for carrying out a GLP test at regular intervals

Each titrant is identified in the system by an unambiguous titrant name.

☞ Open the dialog **System/Titrants**.

System / Titrants			
Titrant	Cyl.	Type	Dos.device
0.1 M NaOH	5 mL	IEU	D1/Titrando 2
AgNO3	20 mL	EU	
EDTA	20 mL	DU	
HClO4	5 mL	IEU	D1/Titrando 1
I2	50 mL	IDU	D2/Sample Processor
Na2S2O3	20 mL	EU	
<input type="button" value="New"/> <input type="button" value="Delete"/> <input type="button" value="Edit"/>			

In the **list of titrants** the **name**, **cylinder volume** and **type**, i.e. exchange unit (**EU**) or dosing unit (**DU**) are given for every titrant. Intelligent exchange or dosing units are indicated by **IEU** and **IDU** and shown in green color (magenta if the line has been selected). For intelligent exchange or dosing units that are attached, the **dosing device connection** is shown additionally and – if several control devices are configured – the name of the control device appears as well.

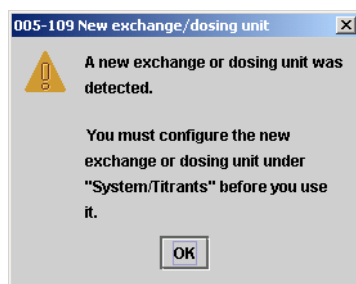
If data is read from the data chip of an intelligent exchange or dosing unit then a check is made whether the titrant list already contains a titrant in the same type of exchange or dosing unit with the same serial number. If this is the case then the older data record will always be overwritten by the new data record, no matter whether the data record in the titrant list of the system or on the data chip is the most recent one.

You can configure a new titrant with **[New]** (see *Section 3.8.1* and *Section 3.8.2*). With **[Delete]** titrants can be removed from the list. Titrant data for intelligent exchange or dosing units can be deleted even when these have just been attached. The data will be entered in the list again the next time that the corresponding unit is attached and the data read out. **[Edit]** opens the dialog for entering titrant data.

3.8.1 Configuring a titrant in a new intelligent exchange or dosing unit

☞ Attach the **new exchange unit** to the Titrando or Dosimat or attach the **new dosing unit** to the Dosino (see manual for the Titrando or for the Dosino).

When the exchange or dosing unit has been recognized the following message will appear:



If you are working with the default settings for the dosing connections then you will also be requested to carry out the "Prep" function in order to rinse all the tubing (see *Section 3.24.2*).

- ☞ Open the dialog **System/Titrants**.
- ☞ Open the **dosing device selection list**, in which new exchange or dosing units are recognized, with **[New]**. Only one dosing device will normally be shown, unless you have attached several new exchange or dosing units.
- ☞ Confirm the selection with **[Select]**.

The dialog in which you can enter the **titrant data** opens automatically.

- ☞ Enter the titrant data as described in *Section 3.8.3*.

3.8.2 Configuring a titrant in a new non-intelligent exchange or dosing unit

A non-intelligent exchange or dosing unit does not need to be attached for the titrant data to be entered.

- ☞ Open the dialog **System/Titrants**.
- ☞ Use **[New]** to open the **dosing device type selection**. Select the exchange unit (for Titrando or Dosimat) or dosing unit (for Dosino).

The dialog in which you can enter the **titrant data** opens automatically.

- ☞ Enter the titrant data as described in *Section 3.8.3*.

3.8.3 Editing titrant data

- ☞ Open the dialog **Titrants/Edit** by either configuring a new titrant (see *Section 3.8.1* and *Section 3.8.2*) or selecting an existing titrant from the list and modifying it with **[Edit]**.



Note!

*If you are using an intelligent exchange or dosing unit and have selected a titrant for a titration or dosing command in the method, then at the START of the determination sequence a check will be made whether you are using the **correct titrant**.*

☞ Enter an unambiguous titrant name under **Titrant** or select a name from the selection list.

☞ Enter the **Concentration** of the titrant and its units.

The titrant concentration can be calculated as the variable **CONC** in the result calculations (see *Section 4.5.1*). This is done by selecting a titrant in the titration command for the method (see *Section 4.1.5*). In a following calculation command you can calculate the concentration of this titrant.

☞ You can add a **Comment** to each titrant.

Normally the **Titer** is determined automatically and assigned. To do this you must draw up a method for the titer determination (see *Section 3.15.2* and *Section 3.16*) and select a titrant in the titration command (see *Section 4.1.5*). In a following calculation command you can assign the variable **TITER** to this titrant (see *Section 4.5.1*). Alternatively you can enter the value for the titer manually. If you alter the titer or the concentration of a titrant in a loaded determination at a later date and would then like to recalculate the determination with the corrected value then you must alter the value in the determination data under **View data/Titrant data** (see *Section 3.18.1*).

☞ You can also enter a **unit** for the titer. This unit is not taken into account in the calculations.

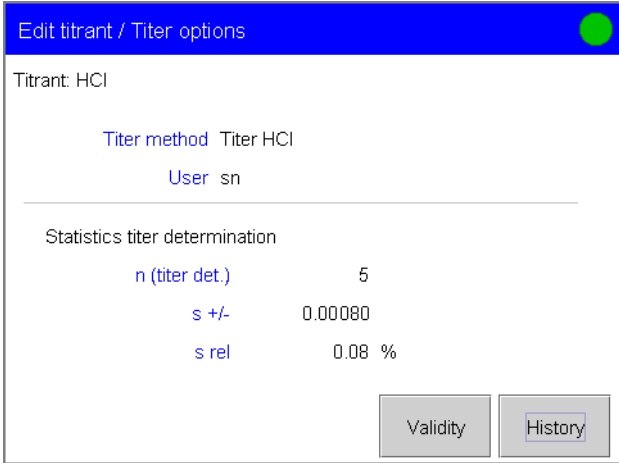
The **date** and time of the **titer determination** are entered automatically on assignment or entry of the titer. If a new titrant is entered then the entry date will be given as the date of the titer determination.

3.8.4 Titer determination options and data

Detailed information about the titer determination is shown under **Titrants/Edit/Titer options**. Under **Titer method** the method with which the titer was determined is shown. If the titer has been entered manually then **manual** will be shown. The user who was logged in when the titer was assigned or entered manually is shown under **User**.

For automatically assigned titers the number of titer determinations is shown together with the absolute and relative standard deviation if the

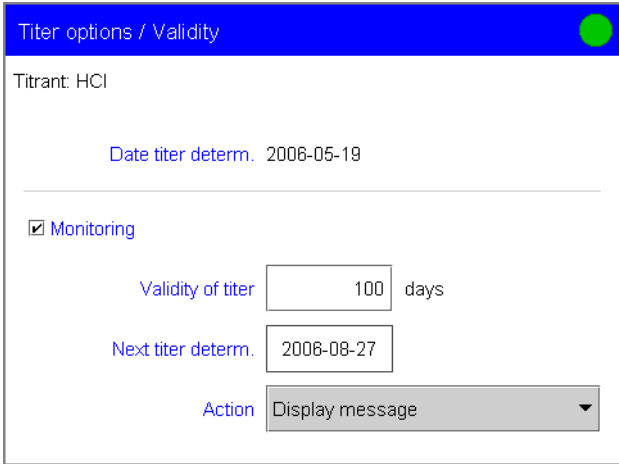
mean value of the determinations has been saved as the titer (see Section 4.5.1).



Statistics titer determination	
n (titer det.)	5
s +/-	0.00080
s rel	0.08 %

You can monitor the **time interval** after which the titrants titer must be redetermined.

☞ Open the dialog **Titer options/Validity** and activate the checkbox for **Monitoring**.

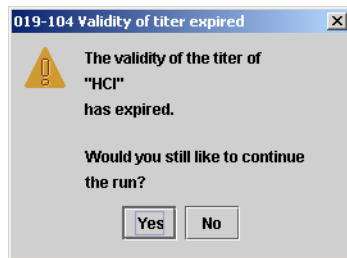


☞ Enter either the **time interval for the validity of the titer** or the **date for the next titer determination**. When either the time interval or the date is edited the other value will be updated automatically.

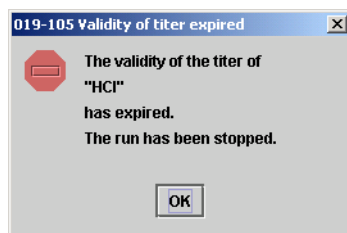
☞ Select an **Action** to be carried out when the time interval has expired. If the titrant is used in the current method then the time interval will be checked at each START of a determination.

When the monitoring interval has expired one of the following **actions** can be selected and carried out:

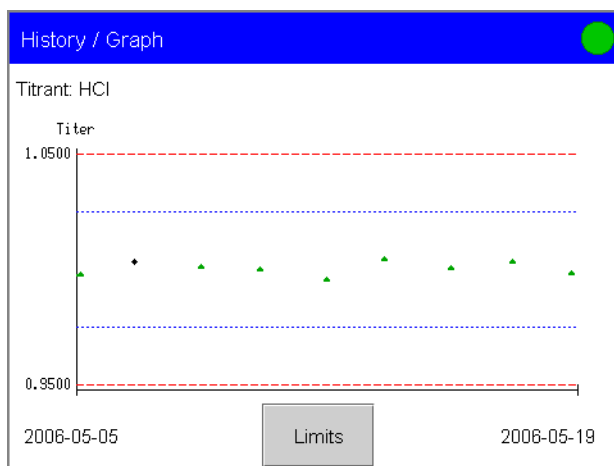
- **Display message:** a message is shown. You can choose whether you want to continue with the determination or cancel the run. If you carry out the run then the fact that the monitoring interval had expired when the determination was carried out will be documented in the determination data. The message can be viewed under **Results/More determination data/Messages** (see Section 3.18.2).



- **Document message:** the fact that the monitoring interval had expired when the determination was carried out will be documented in the determination data. The message can be viewed under **Results/More determination data/Messages** (see Section 3.18.2).
- **Cancel determination:** the determination sequence will be stopped and the following message shown:



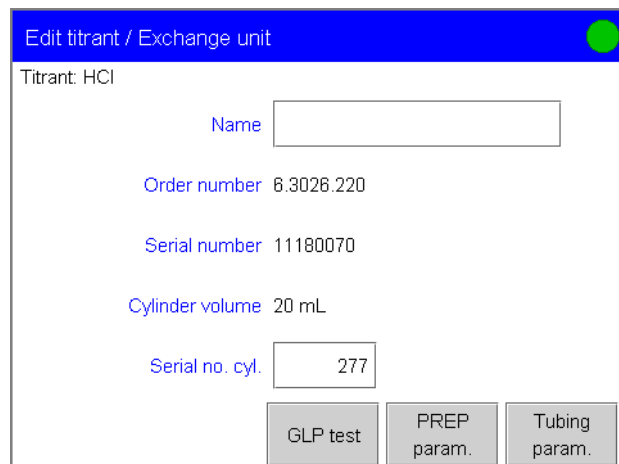
Under **Titer options/History** the date, time and values of the last ten titer determinations are shown in a table. Titrations which have been determined automatically are shown in green, manually entered titer values are shown in black and marked with **(m)**. With **[Graph]** you can open a graph in which the titer values are plotted against the date of the titer determination. With **[Delete history]** you can delete the complete history if, for example, the reagent is changed or a new bottle is opened. If multiple determinations (Statistics) have been carried out in order to calculate the titer then only one entry will be made in the history.



This graph corresponds to a control chart on which both **warning limits** and **intervention limits** are shown for the titer determinations. The values for these warning limits and intervention limits can be entered under **Graph/Limits**. No automatic action is taken when these limits are infringed.

3.8.5 Exchange unit and dosing unit

Under **Edit titrant/Exchange unit** and **Edit titrant/Dosing unit** you can enter data concerning the unit used with the reagent.



The data which can be entered here varies according to whether or not an intelligent exchange or dosing unit is used.

- ☞ You can enter a **Name** for the exchange or dosing unit.
- ☞ The **Order number** and **Serial number** are read out automatically in case of intelligent exchange or dosing units. The data can be entered manually for non-intelligent units.
- ☞ With intelligent exchange or dosing units the **Cylinder volume** is read out automatically. The data can be selected for non-intelligent units. If you have selected a titrant for a titration or dosing command in the method then the **cylinder volume** will be checked during the run. A message will be displayed if the cylinder volume is not the same.



Note!

*If you are using an intelligent exchange or dosing unit and have selected a titrant for a titration or dosing command in the method, then during the run a check will be made whether you are using the **correct titrant**.*

- ☞ With intelligent exchange or dosing units the **serial number of the cylinder** is read out automatically. It can also be entered manually, e. g. after the cylinder has been exchanged. The serial number can be entered manually for non-intelligent units. With new cylinders it is printed on the cylinder.

3.8.6 Tubing parameters and parameters for the preparation procedure

Under **Exchange unit/Tubing parameters** or **Dosing unit/Tubing parameters** you can enter the lengths and diameters of the connected tubing. With the dosing unit you can also alter the port occupancy. These parameters are important for correctly carrying out the **preparation** (PREP command) and **emptying** (EMPTY command) functions for the dosing unit, as the volumes of the tubing connections must be taken into consideration (see Section 3.24.2).

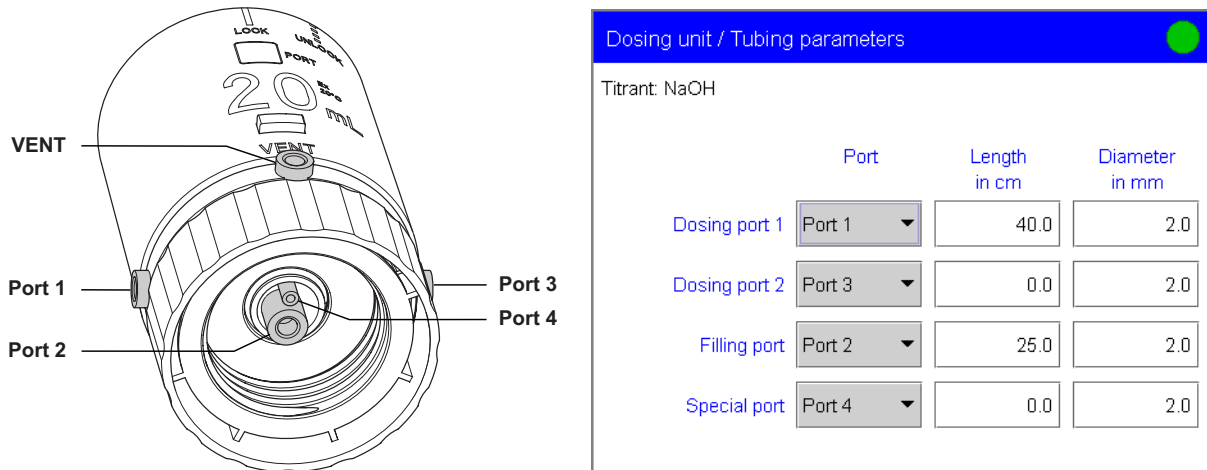


Fig. 3.7: Dosing unit port occupancy and tubing connections

The default values for the **tubing parameters** of the exchange unit and dosing unit have already been entered; these represent the dimensions of the standard tubing supplied. If you do not make any changes to the tubing then you do not need to alter the tubing parameters.

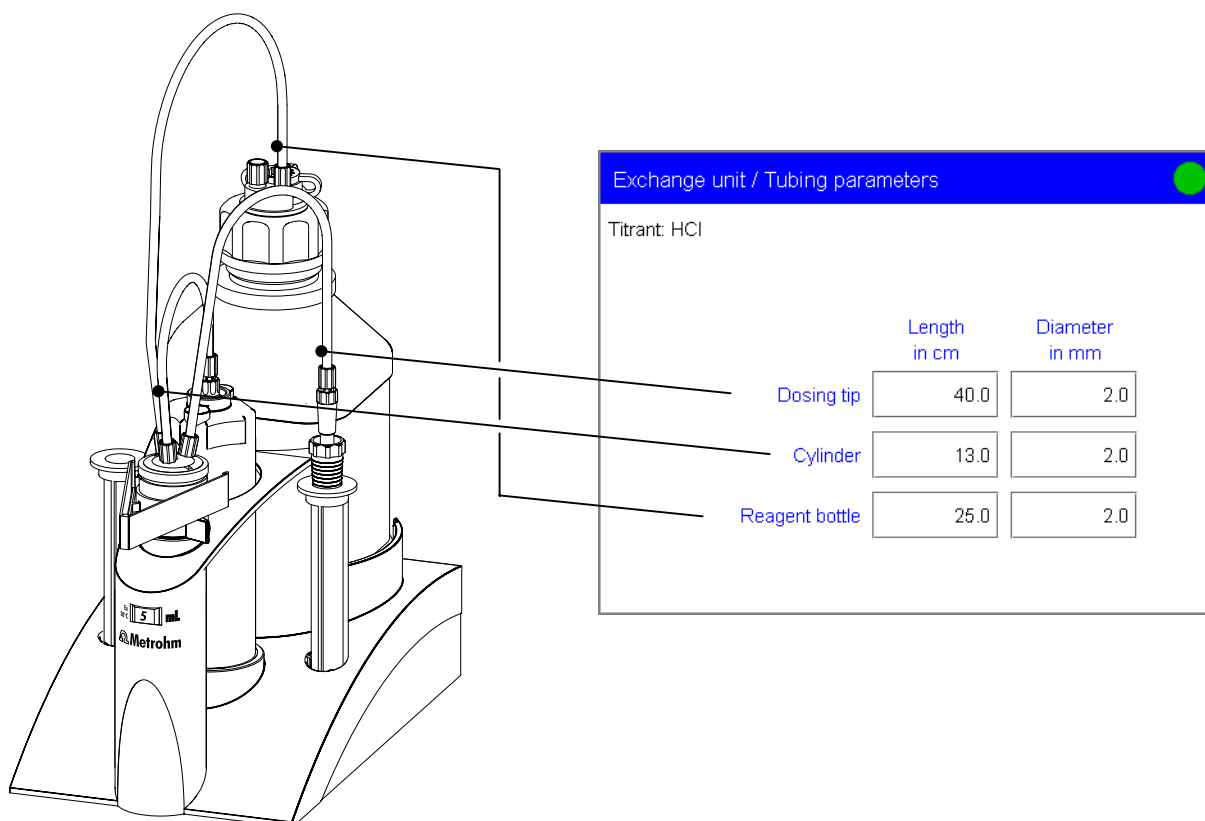


Fig. 3.8: Exchange unit tubing connections

Under **Exchange unit/PREP parameters** and **Dosing unit/PREP parameters** you can enter the parameters for carrying out the **preparation** (PREP command) and **emptying** (EMPTY command; Dosing units only) functions. The preparation function is used to fill bubble-free and to rinse the exchange or dosing units if they have not been used for a long time. When this function has been carried out all the tubing and the cylinder will be filled with reagent. These parameters are different for exchange units and dosing units.

You should carry out the **preparation function** before the first determination or once per day.

Exchange unit

The **preparation function** can be found under **manual control**; which can be started with the **[Manual]** fixed key (see Section 3.24.2). In the **Device manager**, you can define for each dosing device when a message is to be shown to remind you that the PREP function must be carried out for the particular dosing device (see Section 3.10).

Exchange unit / PREP parameters
●

Titrant: HCl

Volume mL

Cycles

Dosing rate mL/min

Filling rate mL/min

- ☞ Enter the **Volume** of reagent which is to be dosed in during a rinsing cycle. The default value is the **cylinder volume**, i.e. the contents of one cylinder is dosed in during a rinsing cycle. You can also enter a different volume.
- ☞ Select the number of **Cycles** to be carried out during the preparation function. At least two rinsing cycles should be carried out in order to remove all the air bubbles.
- ☞ Enter the **Dosing rate** and the **Filling rate** to be used during the PREP function for aspirating and ejecting the reagent. Lower rates should be entered for substances with higher viscosities.

The **maximum dosing rate** and **maximum filling rate** for the exchange unit depend on the cylinder volume:

<i>Cylinder volume</i>	<i>Max. rate</i>
1 mL	3.00 mL/min
5 mL	15.00 mL/min
10 mL	30.00 mL/min
20 mL	60.00 mL/min
50 mL	150.00 mL/min

You can always enter a value between 0.01 and 166.00 mL/min independent of the cylinder volume. When the function is carried out the rate will be reduced automatically to the highest possible value.

Dosing unit

The parameters apply to the **preparation** (PREP command) and **emptying** (EMPTY command) functions. The preparation and emptying functions can be found under **manual control**, which can be started with the **[Manual]** fixed key (see Section 3.24.2). In the **Device manager**, you can define for each dosing device when a message is to be shown to remind you that the PREP function must be carried out for the particular dosing device (see Section 3.10).

Dosing unit / PREP parameters

Titrant: NaOH

Dosing port PREP/EMPTY Dosing port 1

Dosing rate Dos.port 1 maximum ▼ mL/min

Dosing rate Dos.port 2 maximum ▼ mL/min

Dosing rate Filling port maximum ▼ mL/min

Dosing rate Spec.port maximum ▼ mL/min

- ☞ Select the **Dosing port** via which the first cylinder contents are to be ejected during preparation and emptying.
- ☞ Enter the **Dosing rates** for all the ports to be used during the preparation and emptying functions for drawing in and ejecting the reagent. Lower rates should be entered for substances with higher viscosities.

The **maximum dosing rate** and **maximum filling rate** for the dosing unit depend on the cylinder volume:

<i>Cylinder volume</i>	<i>Max. rate</i>
2 mL	6.67 mL/min
5 mL	16.67 mL/min
10 mL	33.33 mL/min
20 mL	66.67 mL/min
50 mL	166.00 mL/min

You can always enter a value between 0.01 and 166.00 mL/min independent of the cylinder volume. When the function is carried out the rate will be reduced automatically to the highest possible value.

3.8.7 Rotating direction of the valve disk (Dosing unit only)

Under **Dosing unit/Valve disk** you can specify the direction of rotation of the valve disk. When choosing **descending** or **ascending** respectively the ports will be moved at in descending or ascending order. The shortest way results with the default setting **automatic**. If you want to define a protected port, then choose **not over** i.e. the valve disk will not be moved over this port. This is especially useful for pipetting functions.

3.8.8 Monitoring the GLP test

You can monitor the **time interval** after which a **GLP test** must be carried out again for the exchange or dosing unit. (A detailed description of the monitoring function using "Titer validity" as an example can be found in *Section 3.8.4.*)

- ☞ Open the dialog **Exchange unit/GLP test** or **Dosing unit/GLP test**. Enter the date of the last GLP test to have been carried out and activate the **Monitoring** checkbox.
- ☞ Enter either the **GLP test interval** or the **date of the next GLP test**. If the time interval or date is altered then the other parameter will be updated automatically.
- ☞ Select an **Action** to be taken when the time interval has expired.

3.8.9 Monitoring the working life

You can monitor the **time interval** after which the **reagent** must be replaced. This is a very good idea when your reagent has a limited working life. (A detailed description of the monitoring function using "Titer validity" as an example can be found in *Section 3.8.4.*) For documentation purposes you can enter the preparation date without monitoring the time interval.

- ☞ Open the dialog **Edit titrant/Working life**. Enter **Preparation date** for the reagent or the date on which the bottle was opened and activate the **Monitoring** checkbox.
- ☞ Enter either the **Working life** or **Expiry date** of the reagent. If the time interval or date is altered then the other parameter will be updated automatically.
- ☞ Select an **Action** to be taken when the working life has expired.

3.9 Sensors

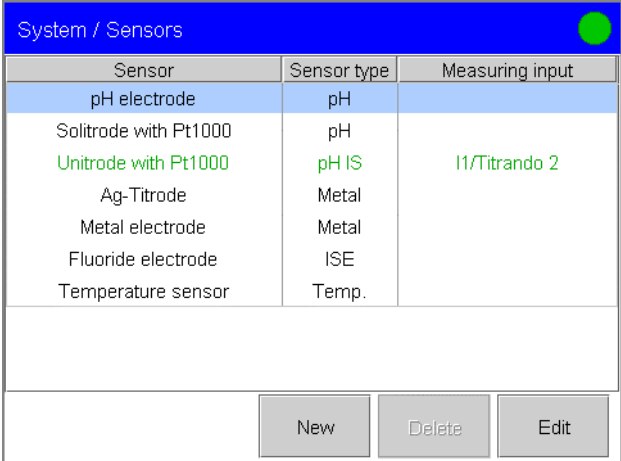
This section describes how you can draw up a list of the sensors used in the system.

The following **sensor data** is stored in the list of sensors:

- Sensor name
- Sensor type
- Order number
- Serial number
- Comment
- Measuring input to which the sensor is connected.
- Calibration data (for pH and ISE sensors only – ISE=Ion-Sensitive Electrode)
- Calibration interval (for pH and ISE sensors only)
- Limit values for the calibration data (for pH and ISE sensors only)
- Working life (with starting date and expiry date)

Each sensor in the system is identified by an unambiguous sensor name.

☞ Open the dialog **System/Sensors**.



Sensor	Sensor type	Measuring input
pH electrode	pH	
Solirode with Pt1000	pH	
Unirode with Pt1000	pH IS	11/Titrando 2
Ag-Titrode	Metal	
Metal electrode	Metal	
Fluoride electrode	ISE	
Temperature sensor	Temp.	

The **name** and **type** of each sensor are shown in the **list of sensors**. Four standard sensors are already defined in the list and cannot be deleted: **pH electrode**, **Metal electrode**, **Fluoride electrode** and **Temperature sensor**. Intelligent sensors are indicated additionally with **IS** and shown in green color (magenta if the line has been selected). When the sensor is connected, the **measuring input** is shown additionally and – if several control devices are configured – the name of the control device appears as well.

If data is read from the data chip of an intelligent sensor then a check is made whether the sensor list already contains a sensor with the same serial number. If this is the case then the older data record will always be overwritten by the new data record, no matter whether the data record in the sensor list of the system or on the data chip is the most recent one.

You can configure new sensors with **[New]** (see *Section 3.9.1*). Sensors can be removed from the list with **[Delete]**. Sensor data for intelligent sensors can be deleted even when they are just connected. The data will be entered in the list again the next time that the corresponding sensor is connected and the data read out. **[Edit]** opens the dialog for entering sensor data.

3.9.1 Configuring a new intelligent sensor

- ☞ Connect the 854 iConnect and the new sensor (iTrodes) as described in the Installation Instructions for the Titrando.

When the sensor has been recognized the following message will appear:



- ☞ Open the dialog **System/Sensors**. The new sensor has been entered in the sensor list though without name.
- ☞ Select the new sensor and press **[Edit]**.

The dialog in which you can enter the **sensor data** opens automatically.

- ☞ Enter the sensor data as described in *Section 3.9.3*.

3.9.2 Configuring a new non-intelligent sensor

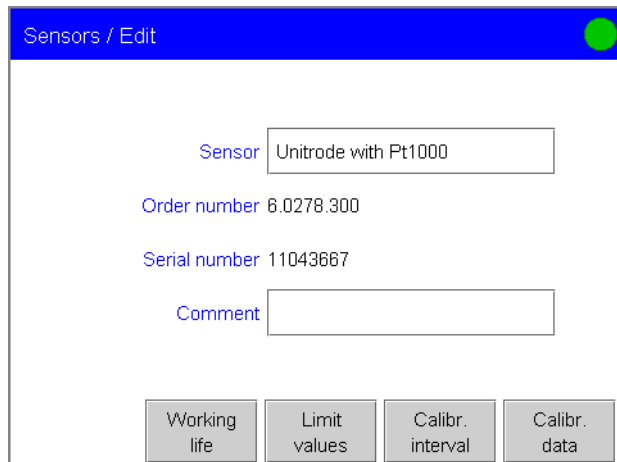
- ☞ Open the dialog **System/Sensors**.
- ☞ Use **[New]** to open the **selection of the sensor type**. Select the sensor type.
- ☞ If you select **ISE electrode** then the ion for which the electrode is selective will be requested automatically. Select the **Ion**. You can also select **Custom** as the ion and then enter a name and select the charge for your "own" ion.

The dialog in which you can enter the **sensor data** opens automatically. The sensor data vary according to the sensor type. Calibration data, calibration interval and calibration data limits are only stored for pH electrodes and ISE electrodes.

- ☞ Enter the sensor data as described in the following section.

3.9.3 Editing sensor data

- ☞ Open the dialog **Sensors/Edit** by either configuring a new sensor (see *Section 3.9.1*) or selecting an existing sensor from the list and modifying it with **[Edit]**.



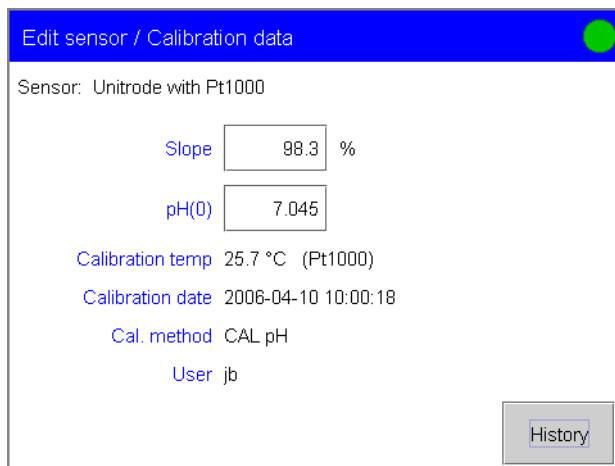
- ☞ Enter an unambiguous name for the sensor under **Sensor**. For ISE electrodes the ion whose concentration can be determined with the sensor is also shown.
- ☞ The **Order number** and **Serial number** are read out automatically in case of intelligent sensors. The data can be entered manually for non-intelligent sensors.
- ☞ You can enter a **Comment** for each sensor.

3.9.4 Calibration data (for pH and ISE electrodes only)

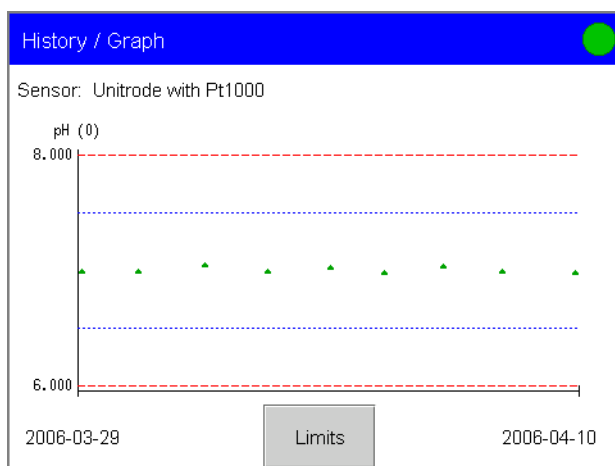
Detailed information about calibrations is given under **Edit sensor/Calibration data**. For pH electrodes the **Slope** is given in % and the electrode zero point **pH(0)** is shown. For ISE electrodes the **Slope** is given in mV; the electrode zero point **E(0)**, the blank concentration **c(blank)** and the variance are also shown. The variance is only calculated, if the calibration has been carried out with at least four standards. The calibration date is entered automatically after a calibration has been carried out (see *Section 4.7*).

Under **Calibration temperature** the temperature at which the calibration was carried out is shown. If the temperature was measured and entered manually during the calibration then this is indicated by **manual**. If the temperature was measured with a connected temperature sensor then the type of sensor (**Pt1000** or **NTC**) will be shown. The **Calibration date** is entered automatically together with the time. When a sensor is entered into the list for the first time the date of entry will be given as the calibration date.

Under **Calibration method** the method used to calibrate the sensor is shown. If the calibration data has been entered manually then **manual** will be shown here. The user who carried out the calibration or entered the calibration data manually is shown under **User**.



Under **Calibration data/History** the calibration data, dates and times of the last ten calibrations are shown in the form of a table. Calibration data which have been determined automatically is shown in green, manually entered calibration data is shown in black and marked with **(m)**. With **[Graph slope]** and **[Graph pH(0)]**, or **[Graph E(0)]** you can open a graph in which the slope or pH(0) for pH electrodes or E(0) for ISE electrodes is plotted against the calibration date. If a sensor has to be replaced then you can delete the complete history with **[Delete history]**.



This graph corresponds to a control chart on which both **warning limits** and **intervention limits** are shown for the calibration data. The values for these warning limits and intervention limits can be entered under **Graph/Limits**. No automatic action is taken when these limits are infringed.

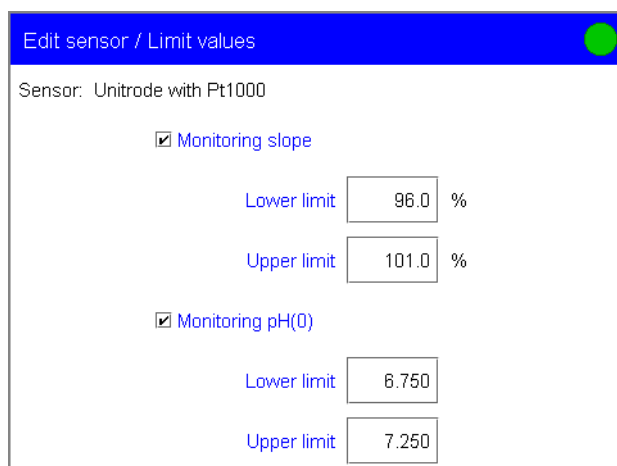
3.9.5 Monitoring the calibration interval (for pH and ISE electrodes only)

You can monitor the **time interval** after which the **sensor** must be **recalibrated**. (A detailed description of the monitoring function using "Titer validity" as an example can be found in *Section 3.8.4.*) For documentation purposes you can enter the starting date without monitoring the time interval.

- ☞ Open the dialog **Edit sensor/Calibration interval** and activate the **Monitoring** checkbox.
- ☞ Enter either the **Calibration interval** or **Next calibration date**. If the time interval or date is altered then the other parameter will be updated automatically.
- ☞ Select an **Action** to be taken when the time interval has expired.

3.9.6 Calibration data limits (for pH and ISE electrodes only)

You can define **Limits** for the calibration data; these will then be monitored when a calibration is carried out (see *Section 4.6*). During the calibration run you can decide whether to accept the calibration data even though the limits have been infringed.



Edit sensor / Limit values
 Sensor: Unirode with Pt1000

Monitoring slope

Lower limit %

Upper limit %

Monitoring pH(0)

Lower limit

Upper limit

- ☞ Activate the checkboxes for the calibration data you wish to monitor (slope, pH(0) or E(0)).
- ☞ Enter the **Lower limit** and **Upper limit** for the calibration data.

3.9.7 Monitoring the working life

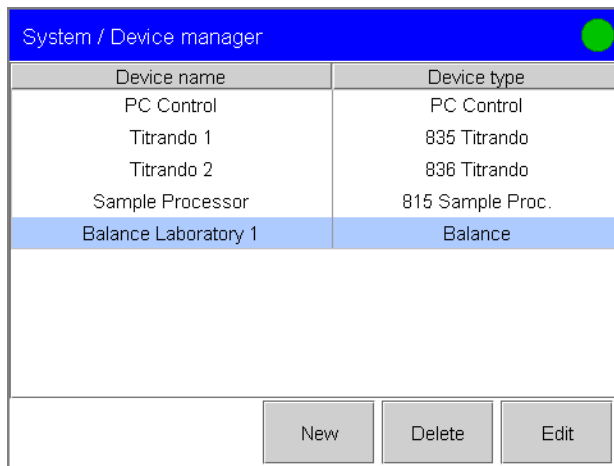
You can monitor the **time interval** after which the **sensor** must be replaced. (A detailed description of the monitoring function using "Titer validity" as an example can be found in *Section 3.8.4*.) For documentation purposes you can enter the starting date without monitoring the time interval.

- ☞ Open the dialog **Edit sensor/Working life**. Enter the date that the sensor was used **for the first time** and activate the **Monitoring** checkbox.
- ☞ Enter either the **Working life** or **Expiry date**. If the time interval or date is altered then the other parameter will be updated automatically.
- ☞ Select an **Action** to be taken when the working life has expired.

3.10 Device manager

This section describes the configuration of the Touch Control, control devices (Titrandos, USB Sample Processor etc.) and the connected peripheral devices. The installation of the hardware is described in the Installation Instructions for the Titrandos. You should first connect all the peripheral devices and then configure them in the device manager.

☞ Open the dialog **System/Device manager**.



The device list gives the name and type of every configured instrument. **PC Control** or **Touch Control**, connected **Titrandos** and a **USB Sample Processor** with the dosing devices, stirrers and remote boxes connected to the MSB are entered automatically in the list. If you are using a Touch Control then the printer, PC keyboard, barcode reader and the RS-232/USB Box will also be automatically recognized and entered in the list with their default settings. The devices used for carrying out a determination are stored together with the determination data (see Section 3.18.4).

You can configure new devices with **[New]** (see Section 3.10.1). **[Delete]** removes devices from the list. Devices which are recognized automatically cannot be deleted from the list while they are still connected. **[Edit]** opens the dialog for entering the device data.



Note!

After you have configured peripheral devices in the device manager you should shut down the system and then restart it.

3.10.1 Configuring a new device

- ☞ Open the dialog **System/Device manager**.
- ☞ Use **[New]** to open the **device selection** window. Select the device type (**Balance**, **Lab Link**, **Barcode reader**, **Titrandos**, **Printer** (Touch Control only), **PC keyboard** (Touch Control only), **Sample Processor**, **Serial ports** (PC Control only) or **RS-232/USB Box** (Touch Control only)). With the exception of the Titrandos (maximum number 3) you can only log in one device of the same type. In this way it is possible to write methods for various Titrandos or a USB Sample Processor even when the hardware is currently not available. The new device is entered in the list.
- ☞ Enter the device data as described in the following section.

3.10.2 Editing device data

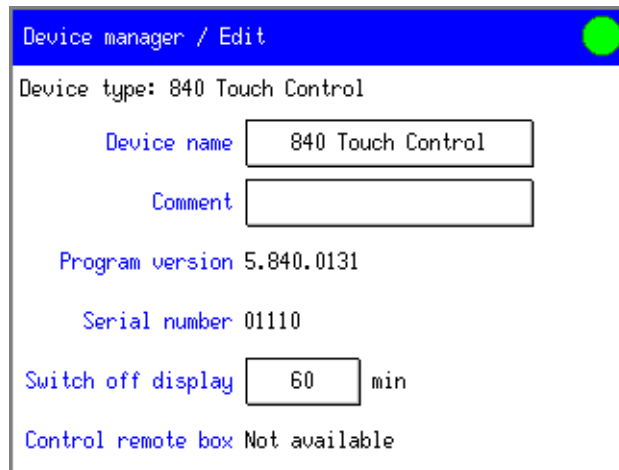
The data stored for a device depends on the type of device.

- ☞ Select the device to be configured from the list and press **[Edit]**.

- ☞ You can enter a **Device name** for each device.
- ☞ You can enter a **Comment** for each device.

3.10.3 PC Control and Touch Control

With the **PC Control** software the **Program version**, the **Serial number** of the USB dongle ("authorization plug") and the **Control remote box** are shown. If no dongle is connected, "demo version" is displayed instead of the serial number. The Control remote box is the interface at which, for example, lines for controlling a Sample Processor during the determination sequence can be set and scanned automatically (see *Section 6.2*). The first remote box to be recognized after system start-up will always be used as the control remote box. Titrandos 1/4 means that the remote box is connected to MSB connection 4 on Titrandos 1 (name of the Titrandos).



With **Touch Control** the **Program version** and **Serial number** of the Touch Control are shown.

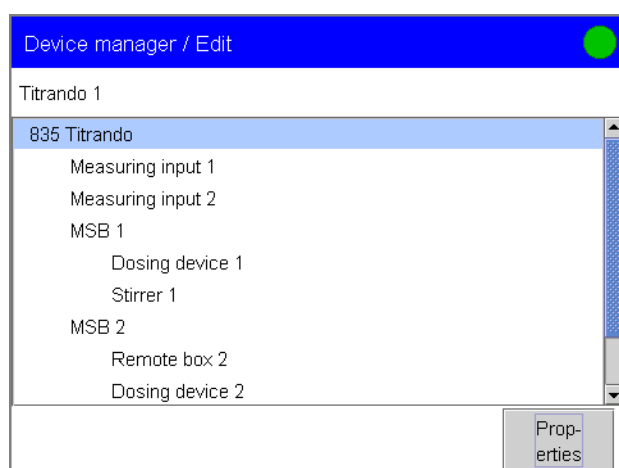
☞ Under **Switch off display** enter the time after which the display illumination is to be switched off automatically when the system has not been used.

As with the PC Control, the **Control remote box** connection is shown.

The **Device name** of the PC Control or Touch Control is printed out in the standard report header.

3.10.4 Titrandos

The measuring inputs and the devices at the MSB connections are listed in a table for the **Titrandos** that are connected. In the following example the Titrando has two measuring interfaces. A dosing device and a stirrer are connected to MSB 1. As this is an 835 Titrando, dosing device 1 is the internal dosing device (see Installation Instructions for the Titrando). A dosing device and a remote box are connected to MSB 2. If the Titrando is not connected, only the **Device name** and **Comment** can be edited.



☞ Select a connection or a device and open the corresponding configuration dialog with **[Properties]**.

The **Program version** and **Serial number** are shown for the **Titrandos** connected.

For the **Measuring inputs** the **ADC type** (Analog-Digital Converter) and **Serial number** of the measuring interface are shown.

- ☞ Select the **Sensor type** for the temperature sensor used at this measuring input. If you use an NTC sensor then you must set two further parameters that can be obtained from the technical specifications of the sensor: the nominal resistance at 25 °C (**R (25 °C)**) and the **B value** referring to measurements of the resistance at 25 °C and 50°C. The default values apply to Metrohm sensors with an NTC sensor. If no B-value is given for your sensor then you can retain the default value. B-values of other NTC sensors are frequently based on different reference temperatures (usually 25 °C / 50 °C – 100 °C). When entering the B-value the influence of the second reference temperature is negligible in comparison with the measuring accuracy of an NTC sensor.

For the **MSB connections** you can define when the request to carry out a **preparation** function (PREP command) for the connected dosing devices is to be displayed. The preparation of the exchange or dosing unit is described in *Section 3.24.2*. For a description of the settings please consult the **online help**.

The **Dosing device type** and the **Serial number** (for type 8xx dosing devices only) are shown for the connected **dosing devices**.

The **Stirrer type** and **Serial number** are shown for the connected **stirrers**.

No properties can be shown or edited for the connected **remote boxes**.

3.10.5 USB Sample Processor and Robotic Titrosampler

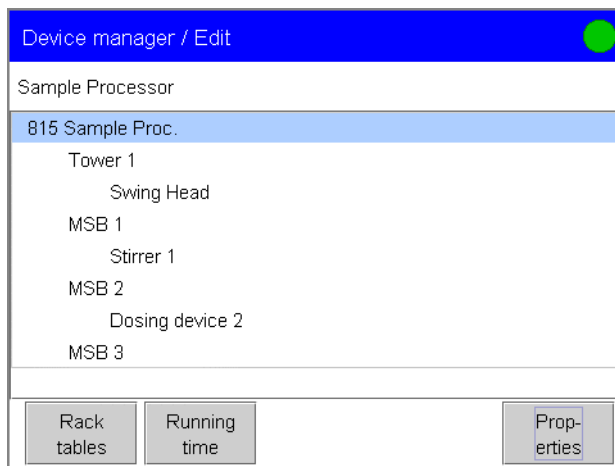


Note!

The following settings apply to all USB Sample Processors.

The Robotic Titrosampler is a USB Sample Processor with a built-in measuring input. The settings of the measuring input are described in *Section 3.10.4*.

The tower (or the towers) and the devices at the MSB connections are listed in a table for the **USB Sample Processor** that is connected. In the following example a stirrer is connected to MSB 1 and a dosing device to MSB 2. If the USB Sample Processor is not connected, only the **Device name** and **Comment** can be edited.



☞ Select a connection or a device and open the corresponding configuration dialog with **[Properties]**.

The settings for the **USB Sample Processor**, the **tower** and the **Swing Head** are described on the following pages.

For the **MSB connections** you can define when the request to carry out the **preparation** function (PREP command) for the connected doing devices is to be displayed. The preparation of the exchange or dosing unit is described in Section 3.24.2. For the description of the settings please consult the **online help**.

The **Stirrer type** and **Serial number** are shown for the connected **stirrers**.

The **Dosing device type** and the **Serial number** (for type 8xx dosing devices only) are shown for the connected **dosing devices**.

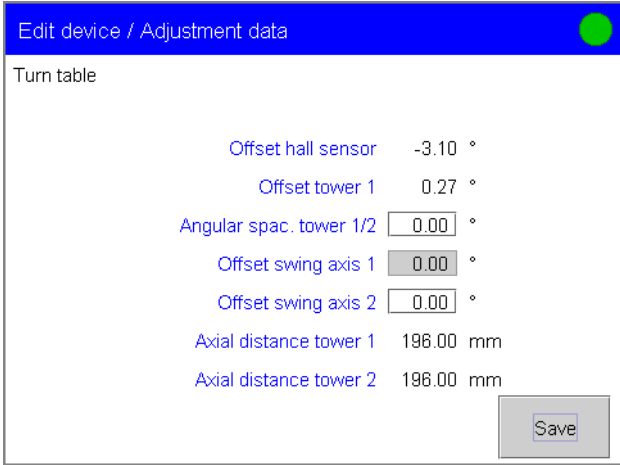
You get to the overview of all the racks available with **[Rack tables]** (see p. 63).

With **[Running time]** you access the overview of the running time meter. The running time meter adds together the time while the USB Sample Processor is "busy" i.e. when a single action is being carried out. After expiry of the time limit set, a message with the advice for a service is displayed. Metrohm recommends to carry out a service after 1000 operating hours. A reset of the running time meter can only be carried out by a Metrohm service technician.

USB Sample Processor

The **Program version**, the **Serial number** and the **name of the current sample rack** are shown for the **USB Sample Processor** connected.

With **[Adjustment data]** you can access an overview of the EEPROM data of the USB Sample Processor.



Turn table

Offset hall sensor	-3.10 °
Offset tower 1	0.27 °
Angular spac. tower 1/2	<input type="text" value="0.00"/> °
Offset swing axis 1	<input type="text" value="0.00"/> °
Offset swing axis 2	<input type="text" value="0.00"/> °
Axial distance tower 1	196.00 mm
Axial distance tower 2	196.00 mm

Save



Attention!

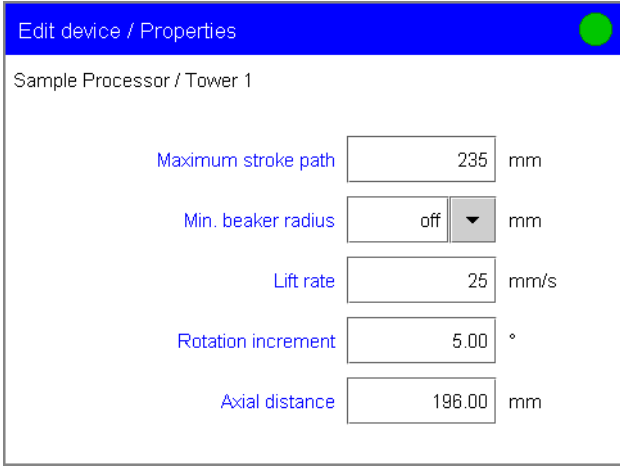
Do not modify these settings under any circumstances. This data is required by the service technician in case of positioning problems.

Tower 1 and 2



Note!

*For a USB Sample Processor with two towers **Tower 1** is the **right-hand tower** when seen from the front and **Tower 2** the **left-hand one**.*



Sample Processor / Tower 1

Maximum stroke path	<input type="text" value="235"/> mm
Min. beaker radius	<input type="text" value="off"/> mm
Lift rate	<input type="text" value="25"/> mm/s
Rotation increment	<input type="text" value="5.00"/> °
Axial distance	<input type="text" value="196.00"/> mm

- Under **Maximum stroke path** you can enter the lowest permissible lift position for automatic and manual operation. This setting of the max. stroke path is important for safety reasons. If this value is set correctly then electrode breakage can be avoided, as a titration

head cannot move to any lower position than the value entered here (0 mm = upper lift stop position).

- Under **Min. beaker radius** you can enter the smallest permissible sample beaker radius for automatic and manual operation. This is also a safety setting in order to prevent a wide, fully equipped titration head from trying to enter a narrow sample vessel. Before the lift is moved to the work position, a comparison will be made between the value entered here and the beaker radius given in the rack table (see p. 63) and, if necessary, an error message will be displayed. There will be no check if no radius has been defined.
- The **Lift rate** can be set for manual operation.
- The **rotation increment** is the angle about which the sample rack should be rotated relatively to the momentary position. This rotation increment is used for the settings **+ rotate** and **- rotate** in the MOVE command.
- The **axial distance** is the distance between the axis of rotation of the sample rack and the swing axis of the robotic arm. This value depends on the model of the USB Sample Processor and is specified in the online help.

Swing Head

Edit device / Properties		
Sample Processor / Tower 1 / Swing Head 786		
Serial number 01110		
Ext. pos.	Angle [°]	Work [mm]
1	60.00	100
2	60.00	0
3	60.00	0
4	60.00	0
<div style="display: flex; justify-content: space-between; align-items: center;"> Ext. pos. 1-4 Robotic arm Adjustm. data Edit </div>		

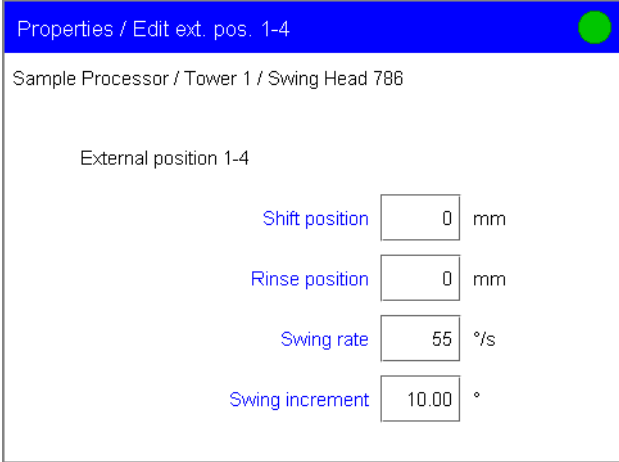
The assigned swing angle and the specific work position are shown for each external position in the properties of the **Swing Head**.

The details of the dialogs **[Ext. pos. 1-4]**, **[Robotic arm]** and **[Adjustm. data]** are described on the following pages.

[Edit] can be used to assign a specific work position and a swing angle to each external position.

External position

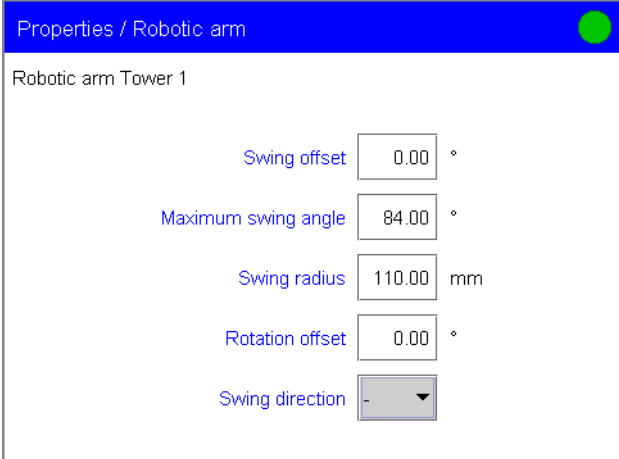
[Ext. pos. 1-4] can be used to assign **shift** and **rinse positions** that are valid for all four external positions.



- The **swing rate** is the rate at which the robotic arm is swung when moving to a rack position, a special beaker or an external position. In manual control and in the command MOVE this rate can be adjusted individually.
- The **swing increment** is the angle about which the robotic arm should be swung relatively to the momentary position. This swing increment is used for the settings **+ swing** and **- swing** in the MOVE command.

Robotic arm

The settings of the robotic arm are listed under [Robotic arm].

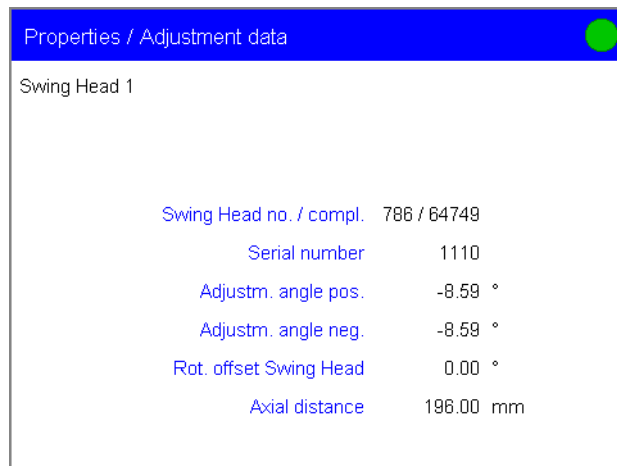


- **Swing offset:** The swing offset is a physical angle offset of a specific robotic arm model. The required values can be found in the leaflet for the robotic arm.
- **Maximum swing angle:** The usable swing range of the robotic arm is defined by this parameter. Because of its construction each robotic arm model has a different value which can be reduced if necessary. The required values can be found in the leaflet for the robotic arm.

- **Swing radius:** The swing radius depends on the length of the robotic arm and together with the axial distance it is the most important parameter for moving accurately to a rack position. The required values can be found in the leaflet for the robotic arm.
- **Rotation offset:** The rotation offset is the offset from the center of the tower to the center of the robotic arm. Normally it does not have to be changed. In case a Swing Head is mounted to the tower with a lateral displacement this value can be determined with a rack adjustment carried out by a service technician.
- **Swing direction:** The swing direction of the robotic arm depends on the type of robotic arm. With a two tower model the robotic arm at tower 1 has to be mounted right-swinging i.e. "-" and left-swinging "+" at tower 2.

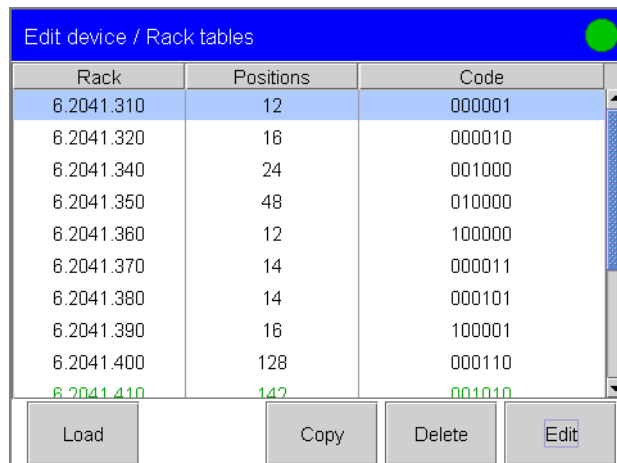
Adjustment data

With **[Adjustment data]** you can access an overview of the EEPROM data of the Swing Head.

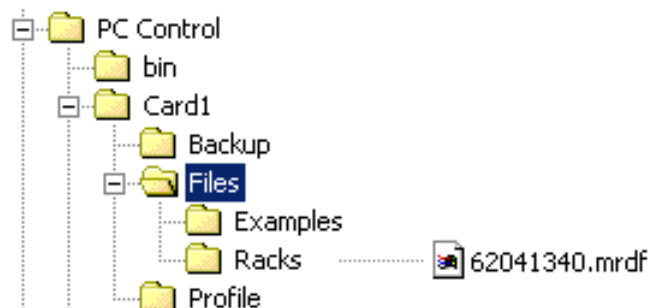


Rack tables

With **[Rack tables]** in the main dialog of the USB Sample Processor you get to the list of all the racks available. The rack currently in position is shown in green. In this dialog window new racks can be loaded or entered and existing ones edited or deleted.



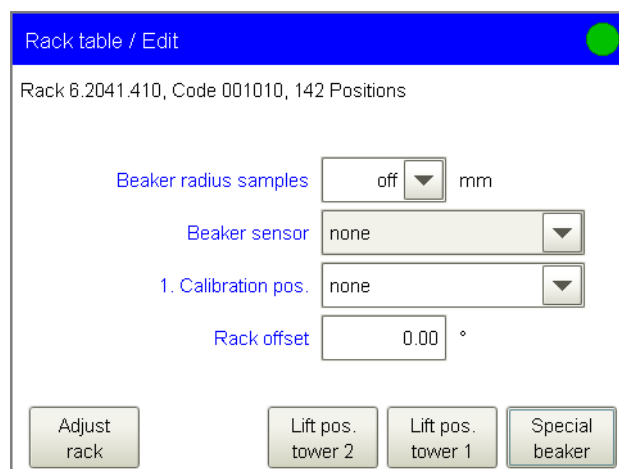
[Load] can be used to load new racks from a card. In PC Control the paths for Card 1 and 2 can be defined in the menu File/Preferences. These may be directories on a hard disk, a network drive or any removable storage medium. With Touch Control Card 1 or Card 2 can only be selected when it is actually in the card slot. The new rack has to be copied necessarily into a subfolder of "**Files**".



If this structure is not complied with, the new rack will not be found because the software accesses directly subfolders of "**Files**".

It is easiest to create your own racks by using the **[Copy]** command to copy an existing rack. In this case it is important that the rack name of the new rack does not already exist. The selected rack code also must not have been assigned already. The proposed rack code "110000" is normally used for special racks.

The selected rack can be adapted with **[Edit]**.



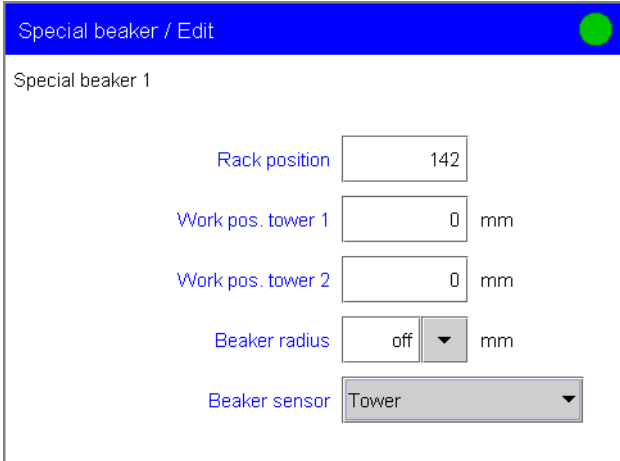
- **Beaker radius samples:** Enter here the actual radius of the sample beakers at the general sample positions of the rack. This beaker radius must not be smaller than the "**Min. beaker radius**" defined in the device properties of the tower (see p. 60). Before the lift is moved to the work position, these two values will be compared and, if necessary, an error message will be displayed.
- **Beaker sensor:** When a sample position is moved to with the MOVE command then, the beaker sensor at the **Tower** or the **Robotic arm** will check whether a sample is present or not. If no beaker sensor has been selected then no check will be made.
- **1. Calibration position** gives the rack position of the first calibration solution for automatic calibration with a USB Sample Processor (see Section 4.7). If a sample position has been given as

the 1st calibration position then it is essential that the other calibration solutions are placed in the directly following rack positions. If special beakers are used for the calibration then there must be as many special beakers defined (see below) as buffers or standard solutions are required for the calibration. The special beakers do not need to be placed in rack positions that directly follow each other.

- **Rack offset:** The rack offset is a tolerance value due to manufacturing between the upper part of the rack and the bottom part. The value is determined by a rack adjustment and displayed here. If necessary it can be edited.
- The rack adjustment is started with **[Adjust rack]**. The procedure is described on page 66.
- Under **[Lift pos. Tower 1]** and **[Lift pos. Tower 2]** the rack-specific lift positions can be defined. These then apply for all rack positions except those that have been defined as special beakers. These positions can be moved to directly under manual control and with the LIFT command. These lift positions can also be assigned directly in manual operation after a move to the required lift height. Only lift positions within the maximum stroke path can be entered. This value is entered in the device properties of the tower. A lift height of 0 mm corresponds to the "Home position", i.e. the lift is being located at the upper stop position.
- **[Special beaker]** is used to specify the positions of the 16 special beakers on the rack.

Special beaker	Rack position
Special beaker 1	142
Special beaker 2	0
Special beaker 3	0
Special beaker 4	0
Special beaker 5	0
Special beaker 6	0
Special beaker 7	0
Special beaker 8	0

☞ Select a special beaker and press **[Edit]**.



- **Rack position:** Each special beaker can be assigned to any rack position. However, they should preferably be assigned to high rack positions so that sample series can be started with rack position 1. Rack positions that have been defined as special beaker positions are no longer available as sample positions.
- **Work pos. Tower 1/2:** A specific work position can be defined for each special beaker. See also Section 3.24.6.
- **Beaker radius:** Enter here the actual radius of the beakers at the special beaker positions of the rack. This beaker radius must not be smaller than the "**Min. beaker radius**" defined in the device properties of the tower (see p. 60). Before the lift is moved to the work position, these two values will be compared and, if necessary, an error message will be displayed.
- **Beaker sensor:** Each time that this special beaker is moved to with the MOVE command then, the beaker sensor will check if a beaker is present. If the sample beaker is missing the method sequence will be halted and a corresponding message will be shown. For the option "**Robotic arm**" a Swing Head must be installed and a suitable work position with beaker contact must be defined for the lift, as this position will be moved to for beaker recognition.

If you exit the edit dialog for the rack table with **[Back]** or **[Home]** then you must confirm the message that appears with **[Yes]** in order for the altered rack data to be transferred to the USB Sample Processor. **[No]** rejects the alterations.

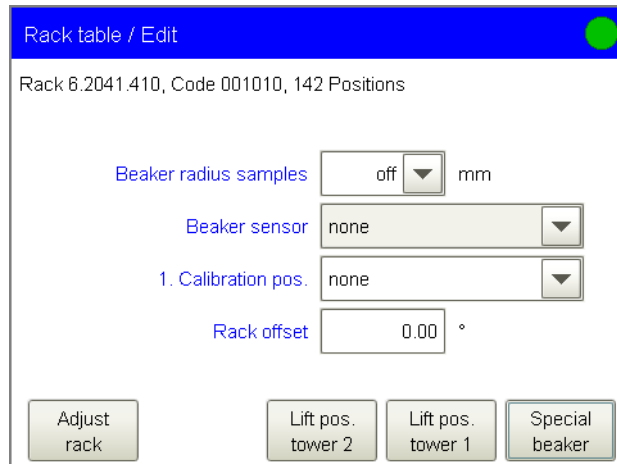
Rack adjustment

If necessary, each sample rack can be finely adjusted, i.e. the rack offset is determined in the direction of rotation. The adjustment of a rack is usually not necessary. However, if the exact positioning of a robotic arm is necessary for a high degree of accuracy (e. g. for very small sample beakers) then a fine adjustment can be carried out. Place the affected rack in position and carry out a rack reset (under manual control). The adjustment is carried out at rack position 1.

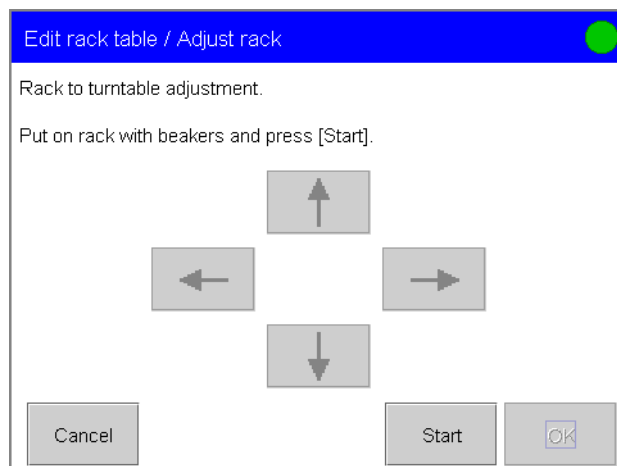
Procedure:

- ☞ Open the dialog **System/Device manager**.
- ☞ Select the USB Sample Processor and press **[Edit]**.

- ☞ Open the list with the available racks with **[Rack tables]**.
- ☞ Select the desired rack and press **[Edit]**.



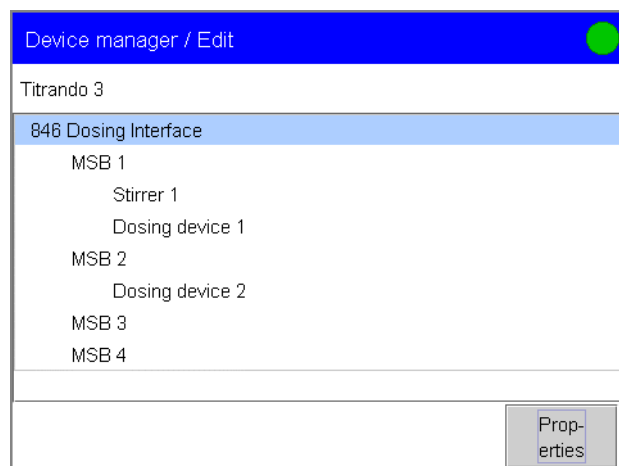
- ☞ Press **[Adjust rack]**.



- ☞ Press **[Start]** (not the green <START> key).
- ☞ The rack is rotated so that rack position 1 is positioned in front of the tower. If a robotic arm is installed, it is swung to rack position 1. The lift then moves to the work position.
- ☞ The position of the lift can now be corrected with the arrow keys **[↑]** and **[↓]**.
- ☞ Now use the **[←]** and **[→]** keys to turn the rack so that the robotic arm or the center of the titration head is positioned exactly above the center of rack position 1.
- ☞ The adjustment is accepted with **[OK]**. The lift is moved to the upper stop position.

3.10.6 Dosing Interface

The devices at the MSB connections are listed in a table for the **Dosing Interfaces** that are connected. A stirrer and a dosing device are connected to MSB 1, a dosing device is connected to MSB 2. If the Dosing Interface is not connected, only the **Device name** and **Comment** can be edited.



☞ Select a connection or a device and open the corresponding configuration dialog with **[Properties]**.

The **Program version** and **Serial number** are shown for the **Dosing Interfaces** connected.

For the **MSB connections** you can define when the request to carry out a **preparation** function (PREP command) for the connected dosing devices is to be displayed. The preparation of the exchange or dosing unit is described in *Section 3.24.2*. For a description of the settings please consult the **online help**.

The **Stirrer type** and **Serial number** are shown for the connected **stirrers**.

The **Dosing device type** and the **Serial number** (for type 8xx dosing devices only) are shown for the connected **dosing devices**.

3.10.7 Printer (Touch Control only)

A **printer** can only be configured for the **Touch Control**. When a printer is connected it is automatically entered in the device list with default parameters. Printer models which can be currently connected can be found on the Internet under www.titrando.com.

- ☞ Select the **printer type**.
- ☞ Select the **paper format** (DIN format **A4** or US format **Letter**).
- ☞ Deactivate the **Color** checkbox if your printout is to be black/white (not for HP LaserJet).
- ☞ Deactivate the checkbox **Compression** in case of faulty reports. The compression enables a faster data transfer to the printer.

☞ Activate the checkbox **Spooler** in order that the Touch Control is not blocked by printing out a report so that you can continue working.



Note!

The Touch Control prints the reports with a fixed resolution of 300 dpi. If you are using a printer with a resolution of 360 dpi (or a multiple, e. g. Epson) then the text will be printed out somewhat smaller than with printers with a resolution of 300 dpi (or a multiple, e. g. Canon or HP).

3.10.8 Balance

Connecting a **balance** to the Titrande or PC is described in the Installation Instructions for the Titrande. In the device manager you must configure the serial interface used to connect the balance.

☞ Select the **Balance type**.

The following table shows the balance type to be selected for various **balance models**:

<i>Balance</i>	<i>Balance type</i>
AND	AND
Mettler AB, AG, AM, PM, XP, XS	Mettler
Mettler AT	Mettler AT
Mettler AX, MX, UMX, PG, AB-S	Mettler AX
Ohaus Voyager, Explorer, Analytical Plus	Ohaus
Precisa	Precisa
Sartorius	Sartorius
Shimadzu BX, BW	Shimadzu

PC Control:

☞ Under **RS-232** select the RS-232 interface (COM) of the PC to which the balance is connected. All the COM interfaces of the PC will be shown.

☞ Add, if not present already, the virtual device **Serial ports** to the device manager and open the list with the available RS-232 interfaces with **[Edit]**. Select the interface to which the balance is connected. Open the dialog with the port parameters with **[Edit]** and configure these. The settings on the balance must agree with these settings here. A description of the parameters can be found in the **online help**.

Touch Control:

- ☞ Under **RS-232** select the RS-232 interface at the RS-232/USB Box which is used to connect the balance.
- ☞ Select the **RS-232/USB Box** in the device manager and open the list with the available RS-232 interfaces with **[Edit]**. Select the interface to which the balance is connected. Open the dialog with the port parameters with **[Edit]** and configure these. The settings on the balance must agree with these settings here. A description of the parameters can be found in the **online help**.

**Note!**

In case of communication problems you can try using the software handshake.

The sample size is transferred as a number with up to ten places, sign and decimal point. Units transmitted by the balance will also be transferred. Control characters will not be transferred. With some balances it is also possible to transmit the sample identification and method from the balance as well as the sample size. When editing the sample data in the sample data silo all the data can be transmitted from the balance (see Section 3.19.3). In some cases a special input unit may be necessary; this can be supplied by the balance manufacturer.

In order to do this the following addresses for the identifications and methods must first be selected:

<i>Balance</i>	<i>Method</i>	<i>Identification 1</i>	<i>Identification 2</i>
Sartorius (input unit)	METH or 27	ID.1 or 26	ID.2 or 24
Mettler AT (input unit)	D (Mthd)	C (ID#1)	B (ID#2)
Mettler AX	Label for ID which contains the method name: METHOD	Label for ID which contains Identification 1 : ID1	Label for ID which contains Identification 2 : ID2

3.10.9 Bluetooth devices

Connecting a **Bluetooth USB adapter** to the Titrandu is described in the Installation Instructions for the Titrandu. In the device manager you must configure the Bluetooth adapter used to connect the device.

- ☞ Look for all the devices within reach with **[Find device]**. If they are switched on, they are entered with status **ok**. Devices which are not switched on at the moment but once have been assigned to a printer or a RS-232 interface are entered with status **not available**.

Device manager / Edit		
Device name	Status	Assignment
BELKIN_PRT_407A80	ok	not defined
Bluetake BT210	ok	not defined
DM-NB	ok	not defined

- ☞ Select the adapter connected to the printer or the balance and open the properties dialog with **[Edit]**.

Edit device / Assignment	
Bluetake BT210	
Bluetooth address	00:08:F4:24:03:67
Device type	Imaging
Profile	Rend;Obj.Tx
Assignment	not defined ▼

- ☞ Select the assignment **Printer** or **COM1...X**.



Attention!

If you change the assignment of a Bluetooth adapter, the Touch Control has to be switched off and on again in order to accept the change.

You have to configure the printer in the device manager.

- ☞ Add a printer to the device manager and configure it as described in Section 3.10.7.



Note!
The **spooler** should be **switched on** to prevent the Touch Control or the printer from getting blocked (see properties dialog of the printer). In the report options, switch on the **printing of the frame** in order to accelerate the printing.

3.10.10 RS-232/USB Box / Serial ports

You can adjust the parameters at the connected RS-232/USB Box or the RS interfaces of the PC respectively under **Edit device/Port parameters**. The parameters are described in the online help.

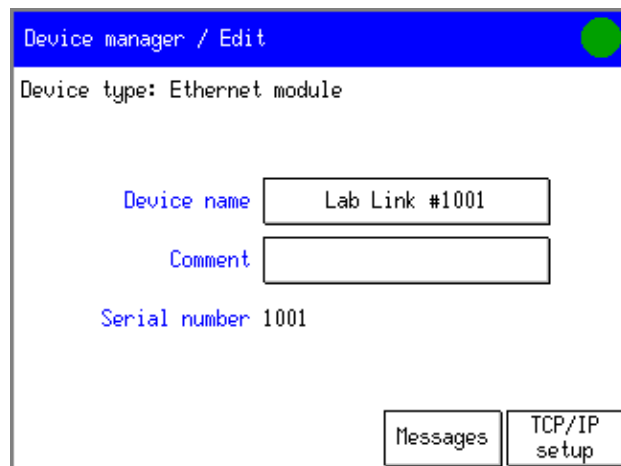


Note!
The Touch Control has to be switched off and on again and the PC Control needs to be restarted in order to accept changed settings.

3.10.11 847 USB Lab Link (Touch Control only)

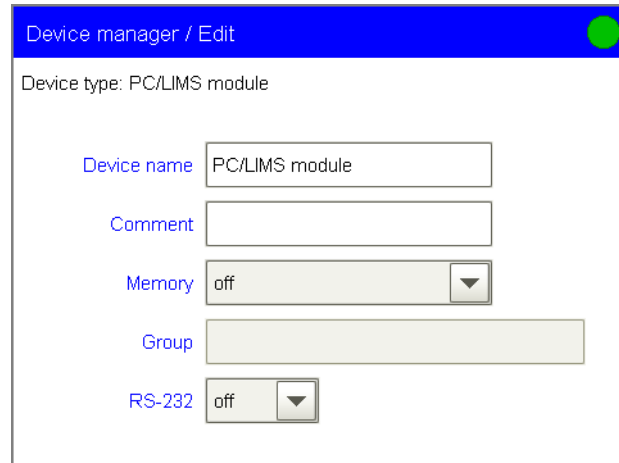
The Touch Control can be connected to a computer via Ethernet using an 847 USB Lab Link. On this computer, a file system can be shared and used as additional memory. Error messages and warnings of the Touch Control can be sent to any receiver via e-mail. The connection and configuration of the 847 USB Lab Link is described in the corresponding Instructions for Use.

The main advantage of the 847 USB Lab Link is that it allows printing on a network printer. The ability of remote control within a network can be used for the "long distance service", i.e. for the support on location of a user by the system administrator.



3.10.12 PC/LIMS module

A machine-readable report containing all the data of a determination (PC/LIMS report) can be saved in a TXT file or sent to a terminal program or a LIMS via an RS-232 interface.



The report is saved or sent either automatically at the end of a determination sequence (see *Section 3.16.10*) or manually with the **[Print]** fixed key (see *Section 3.23.1*). A detailed description of the contents of the PC/LIMS report is given in the Titrando **PC/LIMS Report Guide**.

Save as a text file

In order to save a PC/LIMS report as a TXT file you must configure the system as follows:

- ☞ Select the **Memory** and the **Group** in which the file is to be stored.

Send via a serial interface

In order to send a PC/LIMS report via a serial interface to a terminal program on the PC or directly to a LIMS you must configure the system as follows:

PC Control:



- ☞ Under **RS-232** select the RS-232 interface (COM) of the PC via which the report is to be sent. All the COM interfaces of the PC will be shown.
- ☞ Add, if not present already, the virtual device **Serial ports** to the device manager and open the list with the available RS-232 interfaces with **[Edit]**. Select the interface to which the report is to be sent. Open the dialog with the port parameters with **[Edit]** and configure these. The settings of the interface must agree with these settings here. A description of the parameters can be found in the **online help**.

Touch Control:

- ☞ Under **RS-232** select the RS-232 interface at the RS-232/USB Box to which the computer is connected. The report is sent via this interface.

- ☞ Select the **RS-232/USB Box** in the device manager and open the list with the available RS-232 interfaces with **[Edit]**. Select the interface to which the report is to be sent. Open the dialog with the port parameters with **[Edit]** and configure these. The settings of the interface must agree with these settings here. A description of the parameters can be found in the **online help**.

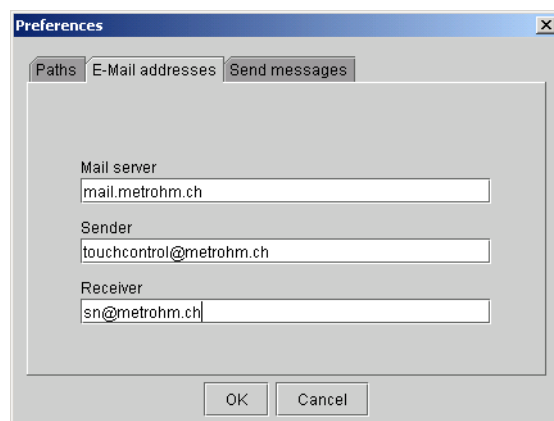
3.10.13 Send messages as e-mails

If you are operating the Titrando system with the PC Control software, you can send messages (all warnings with the symbol  and error messages with the symbol "stop" ) directly from the computer if it has an Internet connection.

You need an 847 USB Lab Link in order to send messages as e-mail from a Touch Control.

Configuration:

- ☞ Open the menu **File/Preferences...**



- ☞ Under **E-Mail addresses**, enter the **Mail server** and the following e-mail addresses: e-mail address to be given as the **Sender** in the e-mail (this address must have the format of an e-mail address, but does not need to be identical to an existing e-mail account); e-mail address of the **Receiver** who is to receive the messages. The **Mail server** can be found in the settings of your e-mail program.
- ☞ Activate the **E-Mail** checkbox under **Send messages**.
- ☞ If the default settings are retained then **messages will only be sent when the system is running** (BUSY), i.e. when a determination or sample series has been started. If you also want to send messages when no analysis is running (READY) then this checkbox must be deactivated.

3.10.14 PC keyboard (Touch Control only)

An external **PC keyboard** can be connected to a Titrand system with Touch Control to make the input of texts easier.

☞ Select the country-specific key occupancy under **Keyboard layout**.

When the PC keyboard is selected the unambiguous identification of the manufacturer (**Vendor ID**) and the **USB address** will be shown automatically.

For entering texts and numbers with the PC keyboard the appropriate text and number input dialog must be opened on the Touch Control. Only the following keys on the PC keyboard have a function :

<i>PC keyboard key</i>	<i>Function in text or numerical input dialog of the Touch Control</i>
Escape	Cancel
Numbers, letters and special characters	Enters the corresponding character
Numbers, letters and special characters + Shift	Enters the corresponding character
Tab (⇧)	Confirms the input and closes the text or numerical input dialog
Backspace, ⌫	Deletes the character in front of the cursor
Delete	Deletes the input
Return (↵)	Starts a new line in multi-line text input
Arrow keys (← →)	Moves the cursor to the left or right by one character
Arrow keys (↑↓)	Moves the cursor up or down by one line in multi-line text input
Numbers and characters on the number block	Enters the corresponding character
Enter on the number block	Confirms the input and closes the text or numerical input dialog

3.10.15 Barcode reader

A **barcode reader** can be connected to the Titrando system to read in sample data or other texts. When a barcode reader is connected to a Titrando system with Touch Control then it is automatically entered into the device list with default parameters. Barcode reader models which can currently be connected can be found on the Internet under www.titrando.com.

- ☞ Select the **Barcode input target** for the barcode character string. For PC Control **Active input field** means that the contents of the barcode will be written into the input field in which the cursor is currently located. With Touch Control **Active input field** means that the barcode string will be written into the **Input field** of an opened text or numerical input dialog. For the input targets **Method**, **Identification 1**, **Identification 2** and **Sample size** (value only) the location can be anywhere in the dialog, the read-in string will be written automatically into the selected input field. Only numerical entries will be accepted for the sample size. Strings which contain characters other than numbers and decimal separators will be ignored.
- ☞ With Touch Control you can also select the country-specific key occupancy for the emulation of the PC keyboard under **Keyboard layout**. This setting must be identical to that on the barcode reader (see barcode reader documentation).

When the barcode reader is connected to a Titrando system with Touch Control then the unambiguous identification of the manufacturer (**Vendor ID**) and the **USB address** will be shown automatically.

When a string has been transmitted by the barcode reader and accepted then this will be confirmed by an acoustic signal. If a Touch Control is used for operating the Titrando system then data should only be read in when the system is in the normal operating status (Ready), i.e. when no determination is running.

3.11 File manager

The file system of the Touch Control and PC Control has the following arrangement:

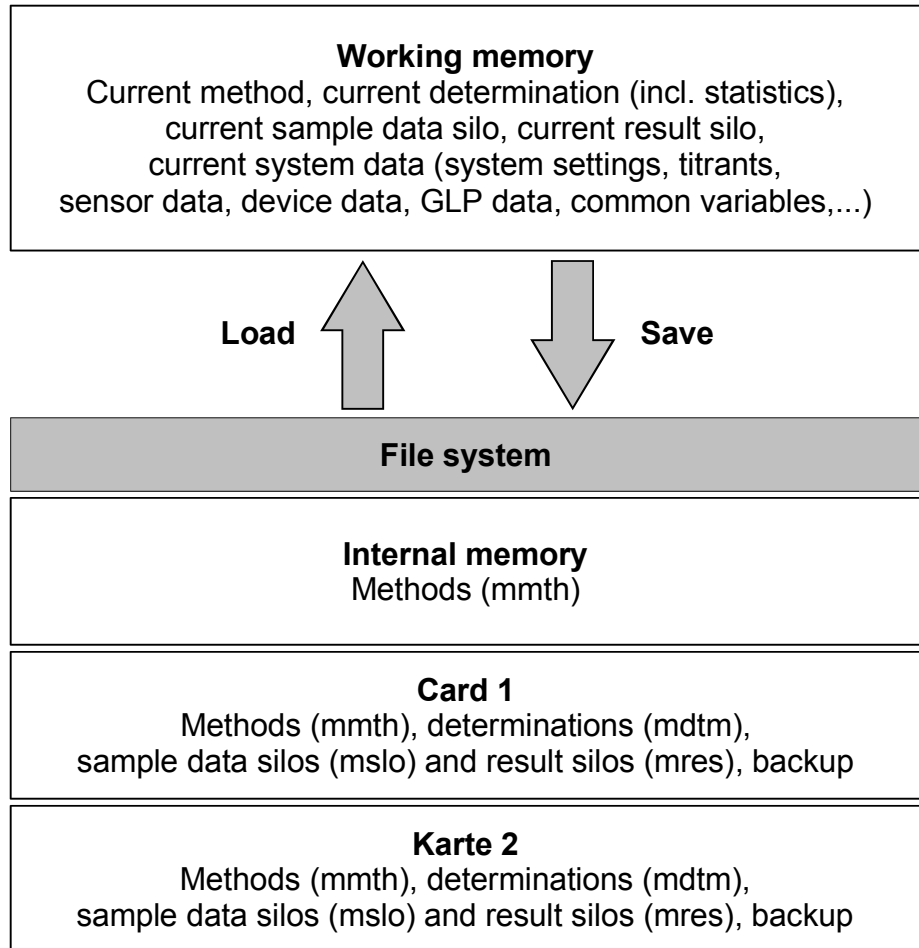
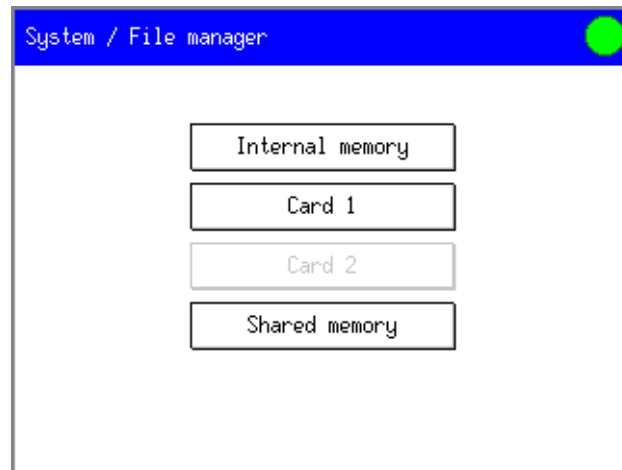


Fig. 3.9: Data memory arrangement

In the **File manager** you can **load, delete, copy, rename and write-protect** methods, determinations, sample data silo files and results silo files as well as edit the **File properties** of each file. You can also produce a **backup** (safety copy) containing all stored data and settings on a card and reload them.

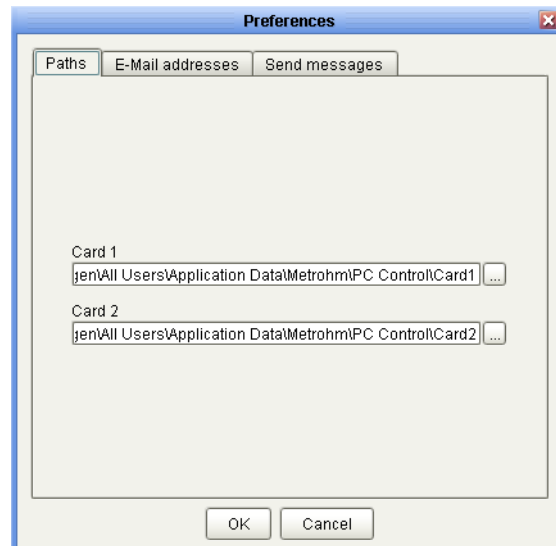
☞ Open the dialog **System/File manager**.



You can select the memory location to be used for the files. **[Card 1]** and **[Card 2]** are inactive when they cannot be accessed. With **Touch Control** the cards must be inserted before you open the file manager. **[Shared memory]** is only visible if an external file system is configured (requires 847 USB Lab Link, see *Section 3.10.11*). If only the internal memory can be accessed then the dialog **System/File manager** will be skipped.

With the **Touch Control** the card slots for the PCMCIA cards are located on the rear of the instrument (see *Fig. 2.2: Rear view of the Touch Control*).

With **PC Control** you can define, on the **Paths** tab, directories for **Card 1** and **Card 2** in the menu **File/Preferences**. These may be directories on a hard disk, a network drive or any removable storage medium. It must be possible to access the drive when the path is being defined.



The example files (**Examples**) are stored in the folder for **Card 1**.



Note!

In **PC Control** the **file groups** correspond to folders. **Card 1** and **Card 2** each have only one level for groups and folders. The file names must be unambiguous for all groups (folders) in a memory location. You should only manage the PC Control files with the file manager of the PC Control software. If you use Windows Explorer for this then there is the risk that you might no longer find the files in PC Control as the folder structure is not compatible.

With **PC Control** if you store files or a backup in the folders selected for Card 1 or Card 2 then the following **Folder structure** will be created automatically:

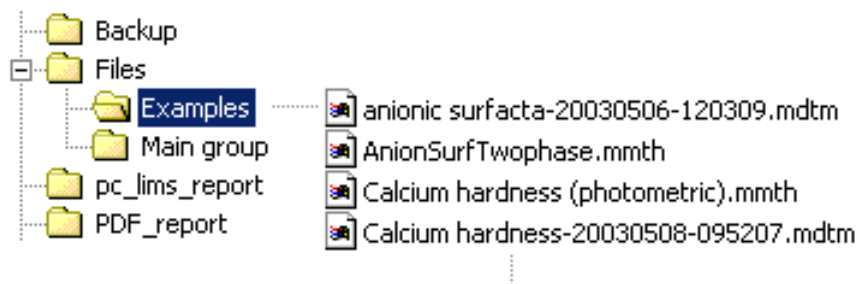
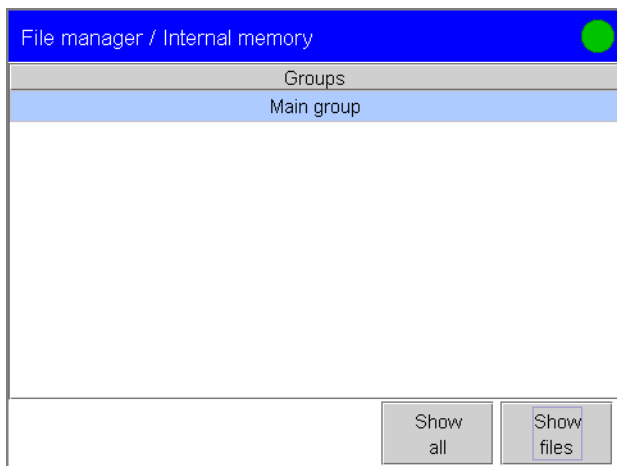


Fig. 3.10: PC Control: Folder structure for Card 1 and Card 2

All the files which belong to a backup are stored in the **Backup** folder. All the files which can be seen in the file manager of the PC Control under **Card 1** and **Card 2** are stored in groups (subfolders) in the **Files** folder. The subfolder (group) **Examples** is present in the standard folder for Card 1 (see above). The example files are stored in this folder. The **Main Group** folder is created as soon as a file is stored without entering a new group. The **pc_lims_report** folder is created when you store a PC/LIMS report as a file without entering a new group. The folders or groups respectively where the PC/LIMS reports are saved are not visible in the file manager. The folder **PDF_report** is generated as soon as a report is saved as a PDF file without changing the path in the menu File/Printer.

All methods which are stored in the internal memory can only be exchanged by using the file manager of the PC Control software. File transfers in the file manager are documented in the audit trail (see Section 3.7.8).

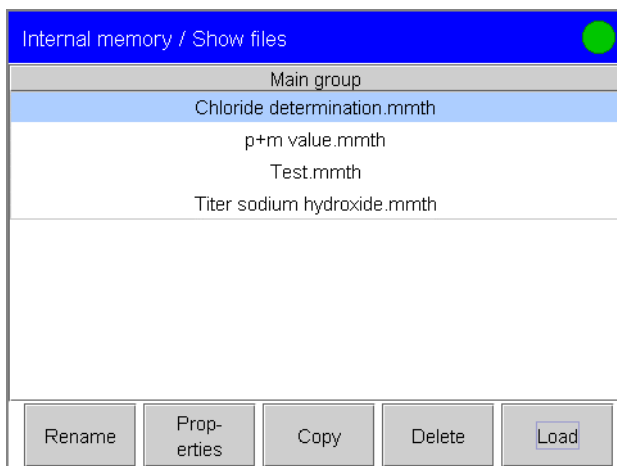
☞ Open the **Internal memory**. The file groups in the internal memory are shown.



You can arrange your files in the **file groups**. The **file names** must be **unambiguous** for each memory location, i.e. you cannot save a file in different groups with the same file name.

From the list of files you can print out a **list with all the files** in these groups with the **[Print]** fixed key.

☞ Open the list of files containing all the files with **[Show all]** or the list of files for the selected group with **[Show files]**. Only methods can be stored in the internal memory. Methods have the file extension **.mmth**.



The selected file is loaded with **[Load]**. The list of files remains open. You can remove the selected file from the list with **[Delete]**. From the list of files you can use the **[Print]** fixed key to print out a **list with all the shown files**.

3.11.1 Copying files

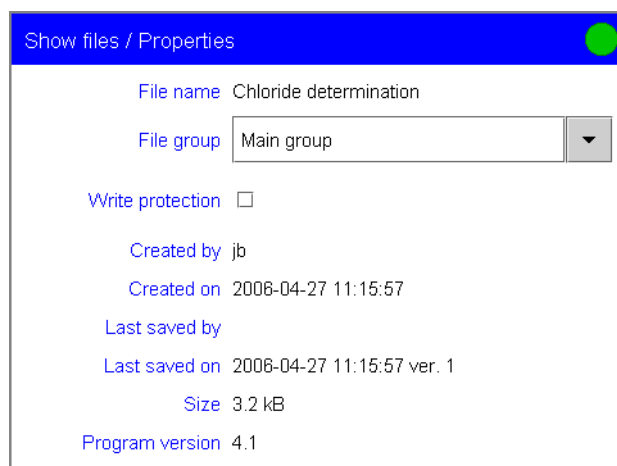
- ☞ Select the file to be copied in the list of files and open the selection of the memory location with **[Copy]**.
- ☞ Select the memory location into which the file is to be copied. The file is copied.

You can only select a memory location that can currently be accessed. If **Card 1** or **Card 2** cannot be accessed then you should exit the file manager and define the path for the card (for **PC Control** – see p. 78) or insert a card into the required card slot (for **Touch Control**) and then copy the file. **[Shared memory]** can only be selected if an external file system is configured (requires 847 USB Lab Link, see *Section 3.10.11*).

The **file group** is retained, i.e. the group will be newly created in the memory location into which the file is copied if it does not already exist there.

3.11.2 File properties

- ☞ Select the file in the list of files whose **Properties** you wish to edit and open the dialog **Show files/Properties**.



Various file properties are shown in this dialog.

- ☞ You can select a different **File group** or enter a new file group in which the file is to be stored. In this way the file can be "regrouped" in the same memory.
- ☞ You can activate **Write protection** for the file. As long as write protection is switched on the file cannot be saved under the same name, deleted, regrouped or renamed. The write protection in PC Control is independent of the write protection in Windows Explorer under Properties.

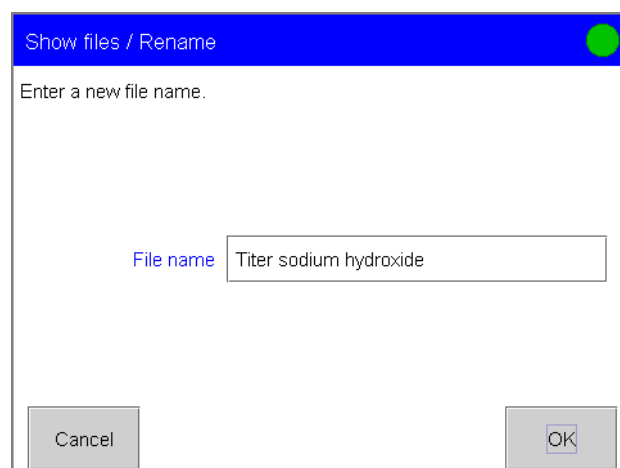
The following data is also shown:

- **User** who **saved the file for the first time**.
- **Date** and time at which **the file was saved for the first time**.
- **User** who was the **last to save the file**.
- **Date** and time at which **the file was saved for the last time**.
- **Version** of the file. The version is increased by one each time that the file is saved under the same file name. The version is retained when the file is copied and loaded in a different system.
- The approximate **Size** of the file in kB.
- **Program version** with which the file was saved for the last time.

File properties can only be printed out in a context-sensitive situation from the dialog **Show files/Properties** with the **[Print]** fixed key.

3.11.3 Renaming a file

- ☞ Select the file to be renamed in the list of files and open the dialog for entering the new file name with **[Rename]**.
- ☞ Enter the new **File name** and confirm with **[OK]**.



Apart from the alteration of the file name the file properties are not affected by the renaming.

3.11.4 Saving a file

Files are saved from the dialogs in which the files can be edited. Saving a file using a method as an example is described below.

- ☞ Open the dialog for saving the file from the main dialog with **[Edit parameters]** and **[Save method]**.

The screenshot shows a dialog box titled "Sequence / Save method". It contains three dropdown menus: "Memory" (set to "Internal memory"), "Group" (set to "Main group"), and "File name" (set to "New method"). At the bottom, there are two buttons: "Cancel" on the left and "Save" on the right.

- ☞ Select the memory location in which the file is to be stored under **Memory**. Methods can be saved in the **Internal memory**, on **Card 1** or **Card 2** or a shared file system (requires 847 USB Lab Link, see *Section 3.10.11*). All other files can only be stored on **Card 1**, **Card 2** or a shared file system.
- ☞ You can arrange your files by storing them in different groups. Enter the **Group** in which the file is to be saved. You can also select the group from the list of existing file groups. If the file has already been saved then the group in which it has been stored will be proposed. The **file names** must be **unambiguous** for each memory location, i.e. you cannot save a file in different groups with the same file name.
- ☞ Enter a **File name**. If the file has already been saved then the name under which it has been stored will be proposed. The file is saved with **[Save]**. The file will not be saved with **[Cancel]** and **[Back]**.

3.11.5 Card 1 and Card 2

Not only methods but also determinations, sample data silo files and results silo files can be stored on **Card 1** and **Card 2**. Safety copies (backups) can also be stored on the cards (see *Section 3.11.6*). The **type of file** can be recognized by the file extension: **mmth** for methods, **mdtm** for determinations, **mslo** for sample data silos and **mres** for results silos.

- ☞ If you are operating the Titrando system with **Touch Control** then insert the **CompactFlash card with the methods** into Card slot 1.
- ☞ Open the **Card 1** memory location. The file groups on Card 1 are shown.

On the cards you can also open lists of files with **[Show all]** or **[Show files]** in exactly the same way as for the internal memory (see *p. 80*).

- ☞ Open the dialog **Card 1/Card info**. Various information about the card is shown in this dialog. Please note that with **PC Control** this information refers to the drive defined under **File/Preferences/Paths**, for example your computer hard disk.
- ☞ You can switch on **Write protection** for the card by deactivating the **Card shared** checkbox. If 'enable' is deactivated it is no longer possible to save, delete and rename files on the card. With **PC**

Control the write protection applies to the folder defined for the card under **File/Preferences/Paths**.

The following information about the card is shown:

- The **Label** of the card or data carrier which was entered when the data carrier was formatted or entered later under Properties in Windows Explorer.
- **Storage capacity** (total space), **Used memory** and **Free memory** for the card, or for the whole data carrier under PC Control.

3.11.6 Backup and restore

You can use the **Backup** function to easily create a safety copy containing all the data and settings of your system.



Note!

Make a **Backup** at **regular** intervals in order to avoid data loss, e. g. caused by voltage variations. For Touch Control we recommend an interval of between one week and one month, depending on how frequently you alter your methods or system settings. For the PC Control software the interval should correspond to the normal data security practice in your company.

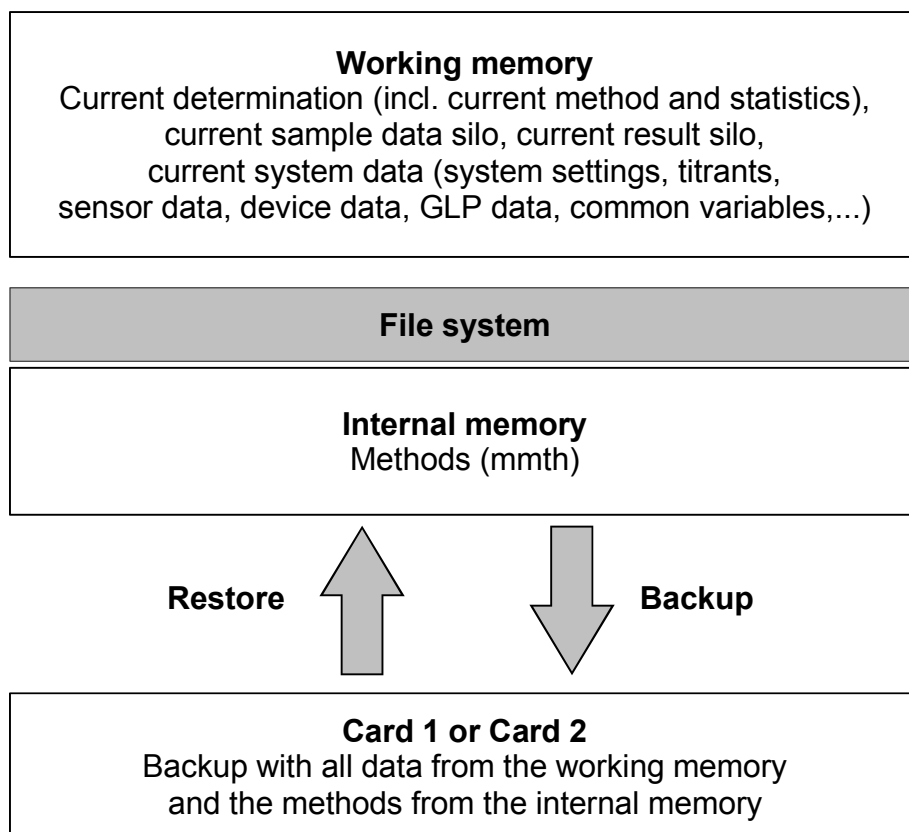


Fig. 3.11: Data transfer Backup/Restore

Touch Control:

☞ Insert the card on which you want to make your safety copy in **Card slot 1 or 2** of the Touch Control.

PC Control:

☞ Select the **directory** or drive on which you want to make your safety copy under **File/Preferences/Paths**.

You can now open the file manager and start the backup.

☞ Open the **Card 1** or **Card 2** memory location in the file manager.

☞ Start data storage with **[Backup]** and answer the query "Do you want to start the backup?" with **[Yes]**.

Only one backup can be stored on each card. If you try to create a new backup on a card which already contains an older backup then this first backup will be overwritten.

You can load the backup data into your system with the **Restore** function. During the backup all your data is saved and, in the restore function, you can select individual data blocks to be loaded from the safety copy.



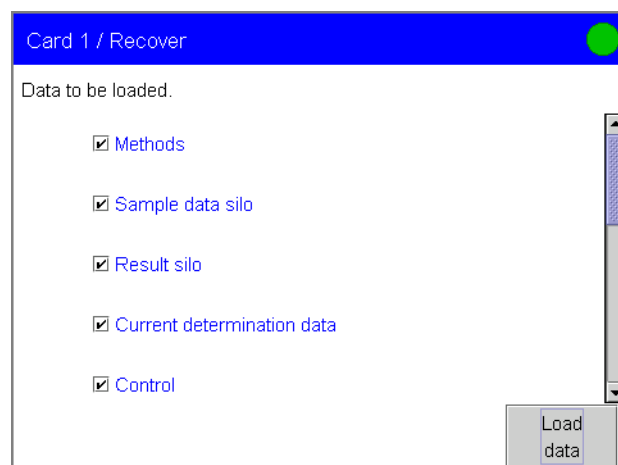
Note!

*During restoring **all** the methods in the internal memory will be deleted.*

Backups are not backwardly compatible, i.e. backups of the latest version cannot be restored with earlier versions.

☞ Open the **Card 1** or **Card 2** memory location in the file manager

☞ With **[Restore]** you can open the dialog for selecting the individual data blocks.



The following data blocks can be loaded individually:

- **Methods** (from the internal memory): all method stored in the internal memory as a file.
- **Sample data silo**: current sample data silo.
- **Result silo**: current result silo.

- **Current determination data:** all the data for the current determination and the current method with which the determination was carried out.
- **Control:** settings under control.
- **User list** under System settings/User administration and settings for each user.
- **System settings/User administration:** all system settings including device-specific dialog configuration and dialog options for the list of commands and fixed keys, device-specific settings for the user administration (login options, password options and audit trail).
- **Titriments:** all titrant data.
- **Sensors:** all sensor data.
- **Device data** (Touch Control only): all data from the device manager. It is not possible to transfer the stored device data from Touch Control to PC Control.
- **GLP data:** all data from the GLP manager. Please note that the GLP data cannot be loaded if you load the safety copy on a different system.
- **Common variables:** all common variables.
- **Templates:** all templates for sample data, result templates, remote lines, custom calibration buffers and report header.
- **Routine dialog settings:** current routine dialog settings under Dialog options/Routine dialog.
- **Sample Processor rack tables:** The racks present in the device manager of the USB Sample Processor.
- **Custom subsequences:** Your own subsequences.
- Deactivate the checkboxes for the data blocks which you do not wish to restore and load the activated data blocks with **[Load data]**.

You can also load a backup from Touch Control in PC Control and vice versa. When a Touch Control backup is loaded in PC Control then the device data is ignored.

- ☞ After the restoring you must shut down the **PC Control software** and then **restart** it, or switch **Touch Control off and then on again**.

3.12 GLP manager

In the **GLP manager** you can document data for various GLP tests. The results of the automatic system tests carried out after START are also documented. You can also draw up a list containing the test tools which you use and enter a service interval for having routine maintenance carried out by a Metrohm service technician.

Further information about quality management and validation is also given in the documentation series **Quality Management with Metrohm** and **Application Bulletin AB 252** (Validation of Metrohm titrators (potentiometric) according to GLP/ISO 9001). An example of a method for carrying out a validation according to AB 252 (**Validation according to AB 252**) is stored under Examples (see *Section 3.15.1*).

☞ Open the dialog **System/GLP manager**.

Test	Last test	Next test
Automat. system test	2006-05-19	Power on
GLP test measurement	2006-01-03	2006-07-03
GLP test titration	2006-01-03	2006-07-03
System validation	2006-01-05	2007-01-08

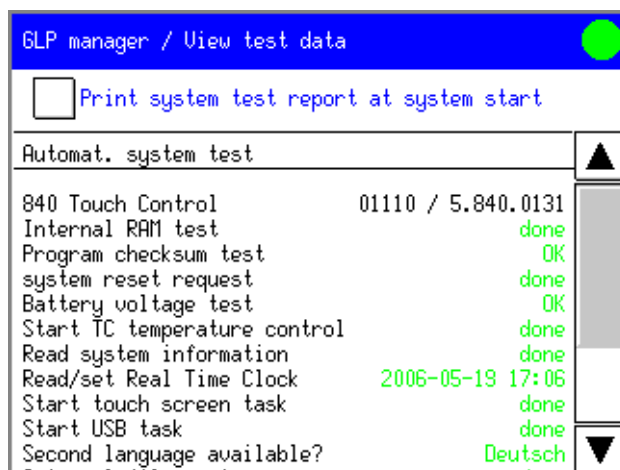
The table shows the last time that each test was carried out and when the next test is to be carried out. A test is entered in the list the first time that it is documented. The following tests can be documented: a **GLP test for measurement**, a **GLP test for titration** and the **system validation**.

You can view the results of the selected test with **[View test data]**.

3.12.1 Automatic system test

The system test is carried out automatically each time that the Touch Control is switched on or each time that the PC Control software is started.

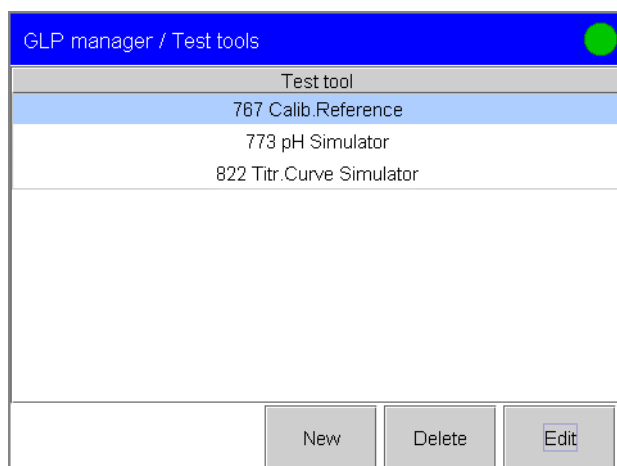
- ☞ Select the line **Automatic system test** in the table and open the results page for the test with **[View test data]**.
- ☞ You can automatically print out the results of the automatic system test each time that the system starts up by activating the **Print system test report at system start** checkbox.



With Touch Control (see example) the test is very comprehensive. The result of each test is shown in **green** if no error has occurred. If a result is shown in **red** then an error occurred when the corresponding test was carried out. Switch the system off and then on again. If the error still occurs please consult Metrohm Service.

3.12.2 Test tools

You can create a **list of test tools** to be used in the tests in the GLP manager.



The list already contains definitions of some test tools.

You can add and edit new test tools with **[New]**. Test tools can be removed from the list with **[Delete]**. The dialog for entering the data for the new tool is opened with **[Edit]**. You can enter a name and comment for each test tool.

3.12.3 GLP tests for measurement and titration

You can document the **GLP tests for measurement and titration** here.

- ☞ Open the dialog **GLP manager/GLP tests HW/SW** (HW = hardware, SW = software).
- ☞ Select **[GLP test measurement]** or **[GLP test titration]** according to which GLP test you wish to document.

The screenshot shows a dialog box titled "GLP tests HW/SW / GLP test measurement". It has a blue header bar with a green circle on the right. The main area contains several input fields:

- Method:** A dropdown menu with "Test measurement" selected.
- User:** A dropdown menu with "jib" selected.
- Test date:** A text box containing "2006-01-03".
- Test result:** A dropdown menu with "Test OK" selected.
- Comment:** An empty text box.

 At the bottom right, there are two buttons: "GLP test interval" and "Hardware".

- ☞ For both tests you can select or enter the **Method** with which the test is to be carried out. Only methods in the internal memory will be shown in the selection list. You can also enter or select the **User** who carried out the test from the selection list.
- ☞ Enter the **Test date** for the last test and select the **Test result**.
- ☞ You can enter a **Comment** for each test.
- ☞ Press **[Hardware]**.

The screenshot shows a dialog box titled "GLP test titration / Hardware". It has a blue header bar with a green circle on the right. The main area contains four dropdown menus:

- Test tool:** "767 Calib.Reference"
- Control device:** "Titrando 1"
- Measuring input:** "1"
- Dosing device:** "1"

- ☞ Select the **Test tool** (list under GLP manager/Test tools), **Control device** (configured in Device manager), **Measuring input** and **Dosing device** (GLP test titration only) used for the test.

You can monitor the **time interval** after which a **GLP test** must be carried out again. (A detailed description of the monitoring function using "Titer validity" as an example can be found in *Section 3.8.4.*)

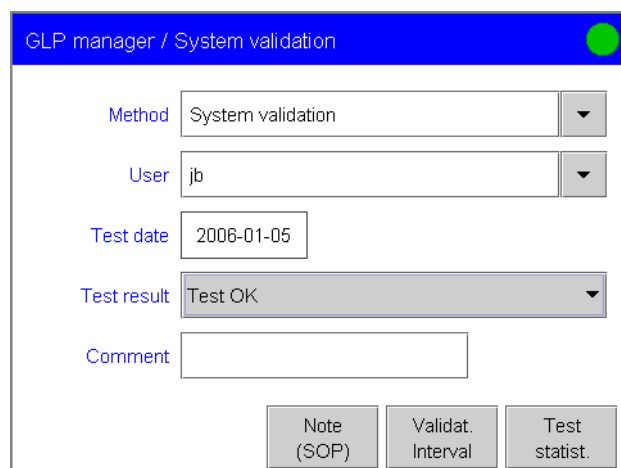
- ☞ Open the dialog **GLP test measurement/Test interval** or **GLP test titration/Test interval**.
- ☞ Activate the **Monitoring** checkbox.
- ☞ Enter either the **GLP test interval** or the date for the **Next GLP test**. If the time interval or date is edited then the other parameter will be updated automatically.
- ☞ Select an **Action** to be carried out when the time interval has expired.

The GLP test interval will always be monitored at the START of a determination.

3.12.4 System validation

You can document the **System validation** results here and also define the time interval after which validation must be carried out again.

- ☞ To document the results of a system validation open the dialog **GLP manager/System validation**.



- ☞ You can select or enter the **Method** used for the system validation. Only methods in the internal memory will be shown in the selection list. You can also enter or select the **User** who carried out the validation from the selection list.
- ☞ Enter the **Test date** for the last validation and select the **Test result**.
- ☞ You can enter a **Comment** for each test.
- ☞ Open the dialog **System validation/Test statistics**. You can document the **statistical data** for the last system validation here. Please consult the **online help** for a description of the individual parameters.

You can monitor the **time interval** after which a **system validation** must be carried out again. (A detailed description of the monitoring function using "Titer validity" as an example can be found in *Section 3.8.4.*)

- ☞ Open the dialog **System validation/Validation interval**.
- ☞ Activate the **Monitoring** checkbox.

- ☞ Enter either the **Validation interval** or the date for the **Next validation**. If the time interval or date is edited then the other parameter will be updated automatically.
- ☞ Select an **Action** to be carried out when the time interval has expired.

The validation interval will always be monitored at the START of a determination.

You can enter a short note under **System validation/Note (SOP)**, e. g. a summary of the SOP (standard operating procedure) according to which the system validation was carried out.

3.12.5 Service interval

You can monitor the **time interval** after which the Titrand system must be serviced again.

- ☞ Choose [**Service interval**] in the dialog **GLP manager/Monitoring**. Enter the date upon which the last service was carried out and activate the **Monitoring** checkbox.
- ☞ Enter either the **Service interval** or date for **Next service**. If the time interval or date is edited then the other parameter will be updated automatically.

When the service interval has expired then the corresponding message will appear at the START of a determination; this will also be documented in the determination data (see *Section 3.18.2*).

3.12.6 Backup interval

You can monitor the **time interval** after which a backup should be carried out.

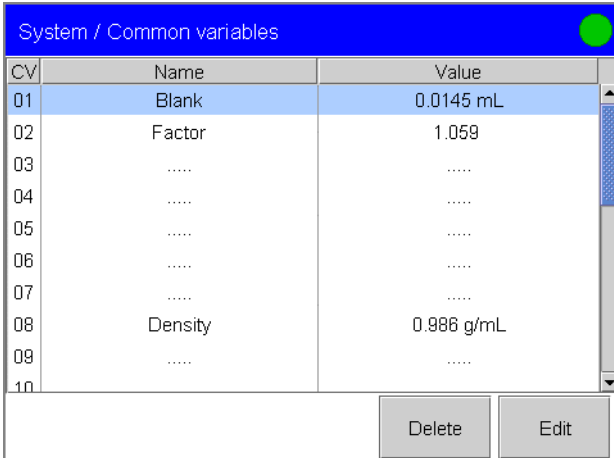
- ☞ Choose [**Backup interval**] in the dialog **GLP manager/Monitoring**. Activate the **Monitoring** checkbox.
- ☞ Enter either the **Backup interval** or the **date for the next backup**. If the time interval or date is edited then the other parameter will be updated automatically.

When the backup interval has expired a corresponding message will appear when the system is started.

3.13 Common variables

Up to 25 **device-specific, method-independent variables** can be stored in the system. These variables can be calculated as **CV01** to **CV25**. Common variables are always used when a result from one determination carried out with Method A is to be used in a determination carried out with Method B. Typical uses are in the determination of a **Blank value** or the content of a standard solution to be taken into consideration when calculating the content in a sample. Common variables can also be automatically requested during the course of a determination (see *Section 4.13.3*). This allows the entry of additional data for the sample which can be used in calculations, e. g. the density, etc.

☞ Open the dialog **System/Common variables**.



CV	Name	Value
01	Blank	0.0145 mL
02	Factor	1.059
03
04
05
06
07
08	Density	0.986 g/mL
09
10

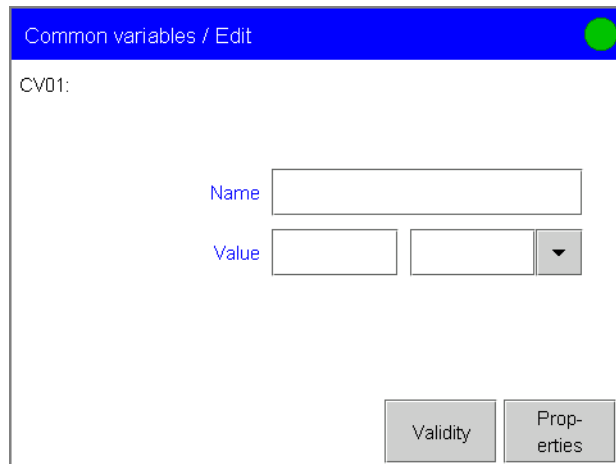
The list of common variables contains the name and values for all 25 common variables. Variables to which no value has yet been assigned are indicated by "....". The selected common variable is deleted with **[Delete]**. **[Edit]** opens the dialog for entering the common variable and monitoring its validity.

3.13.1 Editing common variables

There are three basic ways of editing a common variable: the common variable is edited either under **Common variables/Edit** or entered manually in a **request** in the determination sequence or the variable is automatically assigned to a result in the determination sequence in a **result calculation**.

Editing common variables manually:

☞ Select the common variable to be defined or edited and press **[Edit]**.

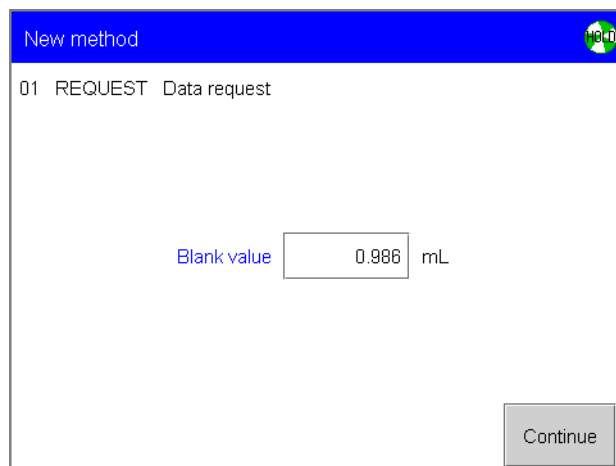


- ☞ Enter a name for the common variable under **Name**.
- ☞ Enter the **Value** and the unit of the common variable.

The name and unit will be shown automatically when the value of the common variable is asked for with a REQUEST command (see below).

Requesting a common variable during a determination sequence:

- ☞ Define a **REQUEST command** in the method as described in *Section 4.13.3*.
- ☞ Define the variable that you want to request (**CV01** to **CV25**) under **Common variable** in the parameter dialog for the REQUEST command. During the determination sequence you can then enter the value of the common variable. The name and unit will be shown in the request. They can be altered under **System/Common variables** (see above).



If you wish to output the common variable as a result then you must define a CALC (calculation) command in the method and calculate a result $RX = CVXX$ (see *Section 4.5.1*).

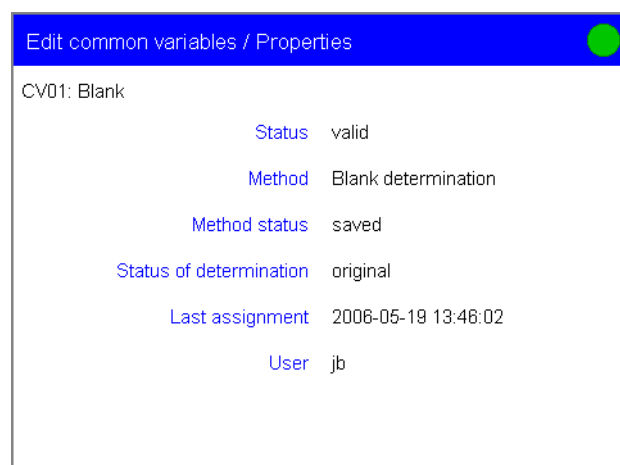
Automatic assignment of a result to a common variable, e. g. for a blank value determination :

- ☞ Define a **CALC (calculation) command** (see *Section 4.5.1*) in the method in which the result (e. g. the blank value) to be assigned to the common variable is calculated. This can also be the mean value of a multiple determination.
- ☞ In the parameter dialog activate the **Save result as common variable** checkbox in the CALC command under **Edit result/Result options** and select the **Variable (CV01 to CV25)** to which the result is to be assigned. The name and unit of the value will also be assigned to the common variable as well as the value.

In further determinations you can use this result (e. g. the blank value) as a common variable (CV01 to CV25, selected as above) in calculations.

3.13.2 Properties of common variables

Under **Edit common variables/Properties** detailed information about the common variables is shown.



The **Status** of the common variable is invalid when no value has been entered or when the time interval for the validity has expired (see *Section 3.13.3*). The method with which the result has been assigned to the common variable is shown under **Method**. If the common variable has been edited manually then **manual** will be shown. **Method status** and **Determination status** are only shown when the common variable is to be assigned automatically in the determination sequence with a CALC command. The date and time of the last alteration of the value of the common variable are shown under **Last assignment**. The user who was logged in when the common variable was assigned or manually edited is shown under **User**.

3.13.3 Monitoring the validity

You can monitor the **time interval** after which the common variable must be assigned a new value. (A detailed description of the monitoring function using "Titer validity" as an example can be found in *Section 3.8.4.*)

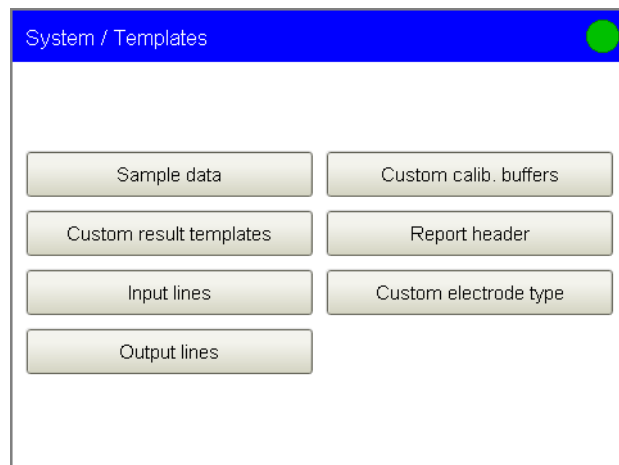
- ☞ Open the dialog **Edit common variables/Validity** and activate the **Monitoring** checkbox.
- ☞ Enter either the **time interval for the validity** of the common variable or the **date for the Next assignment**. If the time interval or date is edited then the other parameter will be updated automatically.
- ☞ Select an **Action** to be carried out when the time interval has expired. The validity of the common variable will be checked on each START of a determination if the particular common variable is to be used in the method.

When the validity of the common variables is being monitored then the date for the **Next assignment** will be shown under **Common variables/Edit**.

3.14 Templates

You can define **system-specific templates** for sample data, result calculations, remote lines, calibration buffers and the report header. You can use these templates when editing the corresponding data.

☞ Open the dialog **System/Templates**.

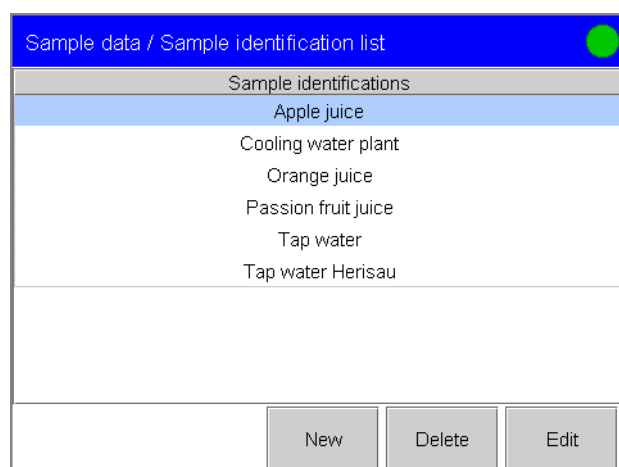


3.14.1 Sample identification list

You can create a system-specific list with templates for sample identifications. You can select from this list when entering the sample data **Identification 1** and **Identification 2** in the main dialog, during a sample data request (REQUEST command) or in the sample data silo (see *Section 3.19*). The **sample identification list** makes it easier for you to enter frequently used sample identifications. It may be a good idea to define the unchanging part of the identification as a template and to add the variable part during sample data input.

☞ Open the dialog **Templates/Sample data**.

☞ Open the list of templates for the sample identifications with **[Sample identification list]**.



☞ Use **[New]** to define all sample identifications which are to be available for selection one after the other.

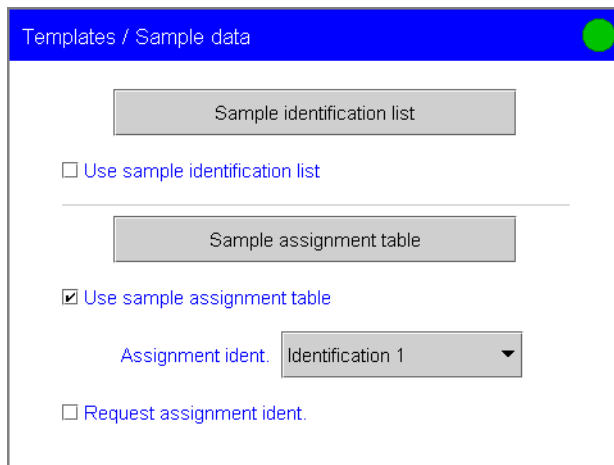
The dialog in which you can enter the templates for **sample identifications** is opened automatically with **[New]**. For an existing template this dialog can be opened with **[Edit]**. Existing sample identifications can be removed from the list with **[Delete]**.

- ☞ Exit the dialog with **[Back]** and activate the **Use sample identification list** checkbox so that you can select from the templates when entering the sample data.

3.14.2 Sample assignment table

If you use the **sample assignment table** then you can be sure that the samples will be processed with the **correct method**. In the sample assignment table a sample identification is assigned to a particular method. Samples with an identification which appears in this table can only be processed by the assigned method. This means that no mistakes can occur. The user enters the sample identification and at the **START** of the determination the correct method is loaded automatically.

- ☞ Open the dialog **Templates/Sample data**.

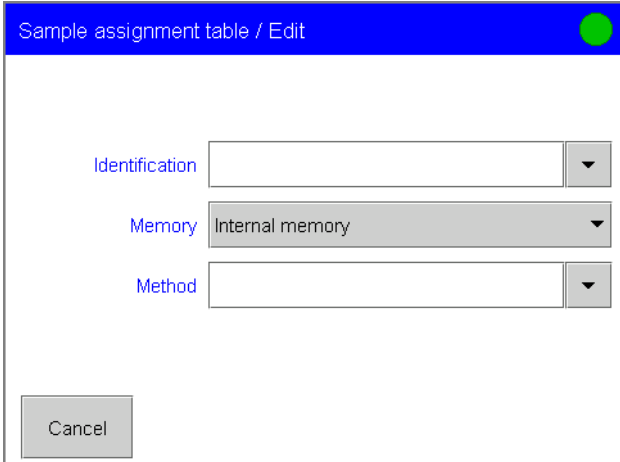


- ☞ Use **[Sample assignment table]** to open the list of sample identifications with their assigned methods.

Sample ident.	Method
Apple juice	Formol number
Cooling water plant *	p+m value
Mineral water	Chloride determination
Orange juice	Formol number
Passion fruit juice	Formol number
Tap water	Water hardness

- ☞ You can define new sample assignments with **[New]**.

The dialog in which you can enter the templates for **sample identifications** is opened automatically with **[New]**. This dialog can be opened with **[Edit]** for an existing template. Existing sample identifications can be removed from the list with **[Delete]**.



- ☞ Enter the **Identification** for the sample assignment. You can also select an identification from the sample identification list (see Section 3.14.1). You can enter an ***** as a wildcard at the beginning or end of the character string. In this way, for example, you can append a running number which will be ignored during the method assignment (see example **Cooling water plant ***). Upper and lower case letters will be differentiated in the comparison.
- ☞ Enter the **Memory** from which the method is to be loaded. Memory locations which cannot be currently accessed can also be selected.
- ☞ Enter the name of the **Method** with which the sample is to be processed. If the method is already stored in the memory selected above then it can also be selected.
- ☞ Exit the input dialog and activate the **Use sample assignment table** checkbox under **Templates/Sample data**. Determinations can now only be carried out when the assignment identification has been entered and is present in the sample assignment table.
- ☞ Choose whether **Identification 1** or **Identification 2** is to be used for the **Assignment identification** in order to load the correct method.
- ☞ You can also request the assignment identification automatically after the START. If the **Request assignment identification** checkbox is activated then the method with which the sample is to be processed will only be loaded when the assignment identification is entered and confirmed with **[Continue]**.



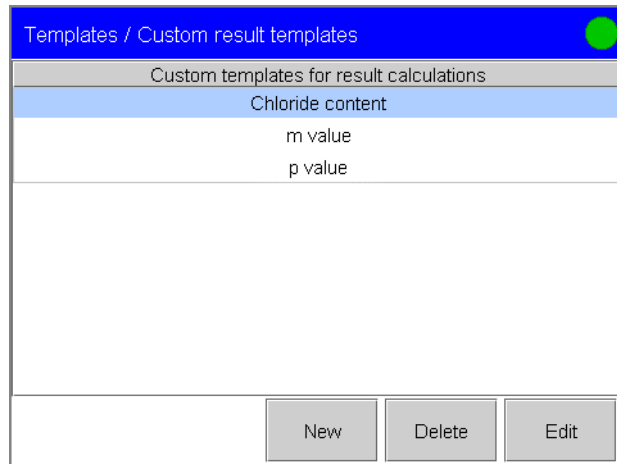
Note!

*If you have activated **Use sample assignment table** then you can no longer define the method to be used for processing the sample in the sample data silo. If methods have already been defined then they will be ignored.*

3.14.3 Custom results templates

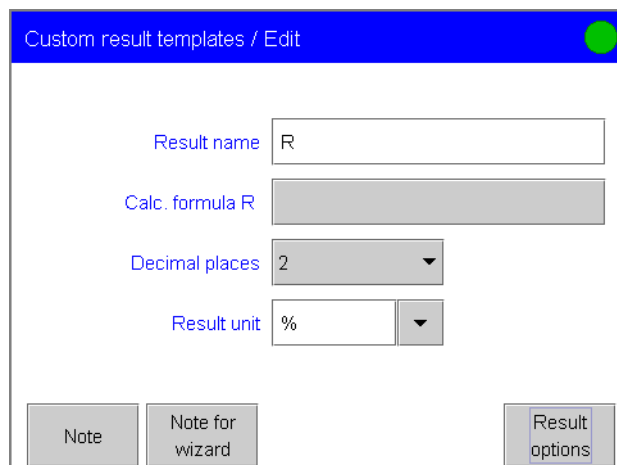
Templates can be created for editing result calculations in the methods; these can be loaded when editing CALC commands.

☞ Open the dialog **Templates/Custom result templates**.



With **[New]** you can define new templates. Existing templates can be removed from the list with **[Delete]** or altered with **[Edit]**.

☞ Use **[New]** to open the edit dialog for a new result template.



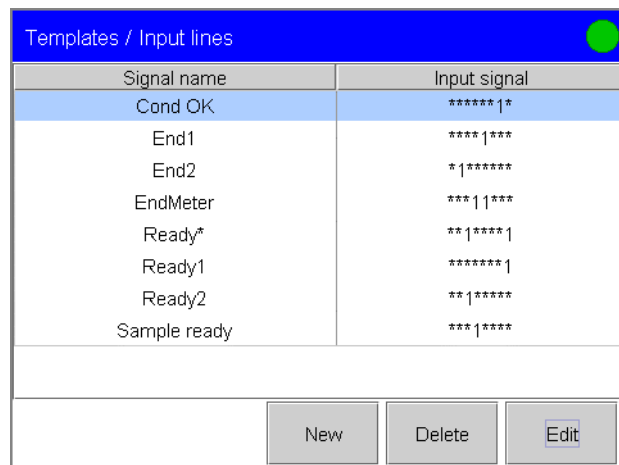
Creating result templates is carried out in the same way as editing the result calculations in the CALC command (see *Section 4.5.1*). A **Note for wizard** can also be entered. This note will be shown when the template is loaded during the creation of a new result in the CALC command.

Further special features when creating result templates are described in *Section 4.5.4*.

3.14.4 Input lines

Binary patterns can be defined for **scanning remote lines** with the SCAN command (see *Section 4.11.1*) during the determination sequence; these can then be selected when editing the parameters.

☞ Open the dialog **Templates/Input lines**.



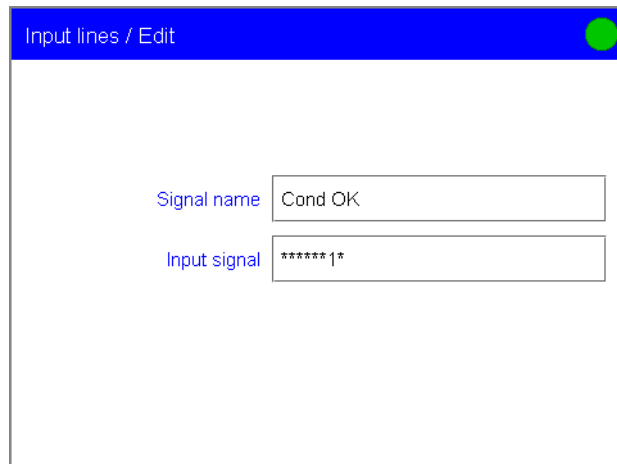
You can define new templates with **[New]**. Existing templates can be removed from the list with **[Delete]** or edited with **[Edit]**.

List of predefined input lines

Parameter	Signal pattern	Function
Cond OK	*****1*	waits for "Cond OK" condition of device 1
End1	****1***	waits for the EOD impulse from device 1 (Titrino, Titrand)
End2	*1*****	waits for the EOD impulse from device 2
EndMeter	***11***	waits for the EOD impulse from ion meter or pH-Meter (stirrer 1 will be switched on during the waiting period)
Ready*	**1****1	waits for "ready" condition of devices 1 and 2 (Titrino, Titrand)
Ready1	*****1	waits for "ready" condition of device 1
Ready2	**1*****	waits for "ready" condition of device 2
Sample ready	***1****	waits for an impulse to continue e. g. of a connected Sample Processor as soon as it is ready

With the parameter **Ready*** it is possible to scan the condition of devices working in parallel. In this case the 'Ready' line of both devices must be statically set (i.e. constantly) at the end of a determination. Devices which only transmit a brief impulse at the end of e. g. a measurement cannot be controlled in parallel.

☞ Use **[Edit]** to open the edit dialog for the template **Cond OK**.

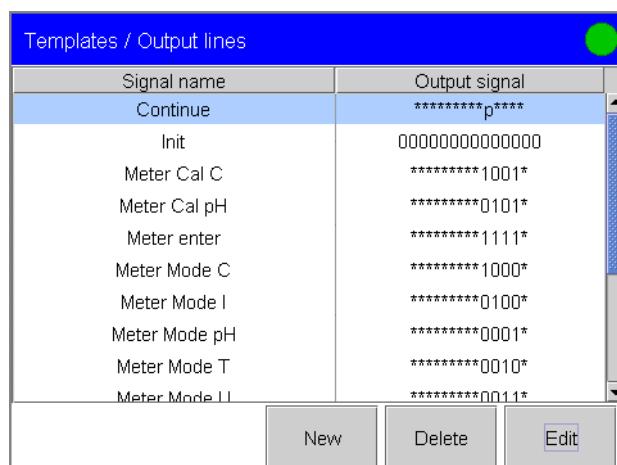


To input the binary pattern please consult the **online help**.

3.14.5 Output lines

Binary patterns can be defined for **setting remote lines** with the CTRL command (see *Section 4.11.2*) during the determination sequence or in manual operation (see *Section 3.24.5*); these can then be selected when editing the parameters.

☞ Open the dialog **Templates/Output lines**.



You can define new templates with **[New]**. Existing templates can be removed from the list with **[Delete]** or edited with **[Edit]**.

List of predefined output lines

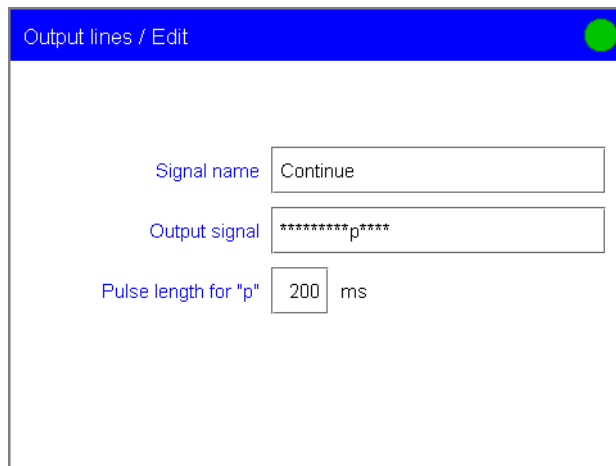
Parameter	Signal pattern	Function
Continue	*****p****	sends a pulse to continue to the connected Sample Processor
INIT	00000000000000	initializes the Remote interface
METER Cal C	*****1001*	switches ion meter to Conc calibration
METER Cal pH	*****0101*	switches ion meter or pH meter to pH calibration and starts it
METER enter	*****1111*	simulates the <ENTER> key for ion meter or pH meter (essential for pH calibration with 691/780/481, in order to start the measurement of the second buffer)

METER Mode C	*****1000*	switches ion meter to Conc measurement
METER Mode I	*****0100*	switches ion meter or pH meter to Ipol (mV measurement) and starts it
METER Mode pH	*****0001*	switches ion meter or pH meter to pH measurement and starts it
METER Mode T	*****0010*	switches ion meter or pH meter to temperature measurement and starts it
METER Mode U	*****0011*	switches ion meter or pH meter to mV measurement and starts it
Start device1	*****p	starts device 1 (e. g. Titrino, Titrando, ...) *)
Start device2	*****p*****	starts device 2 (see above, only with multiple cable)*)
Start device*	*****p****p	starts devices 1 and 2 " *)
Start Dos1	*****p*****	starts Dosimat at device 1 (Titrino via "activate")
Start Dos2	*****p*****	starts Dosimat at device 2 "
Start Dos*	*****p*p*****	starts Dosimat at devices 1 and 2 "

For **START** commands the signal is transmitted as a short impulse of 200 ms.

*) With pH meters or ion meters a result report is triggered

☞ Use **[Edit]** to open the edit dialog for the template **Continue**.

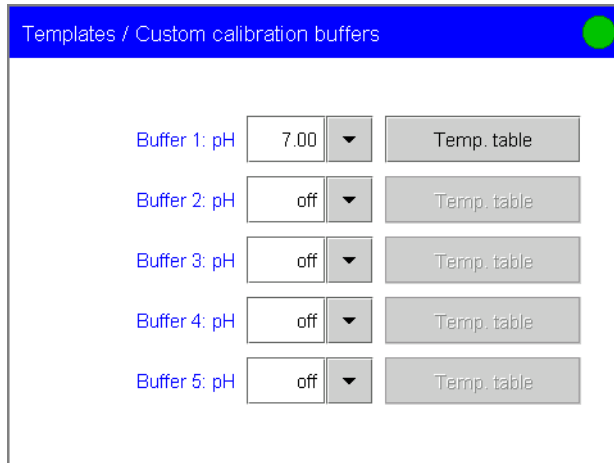


You can also set pulses for the lines by entering a **p** in the binary pattern. The pulse length is defined under **Pulse length for "p"**. The pulse length can only be entered for signals which are defined as templates. If you define a signal directly in the CTRL command or in manual operation then a fixed pulse length of 200 ms will be used. To input the binary pattern please consult the **online help**.

3.14.6 Custom calibration buffers

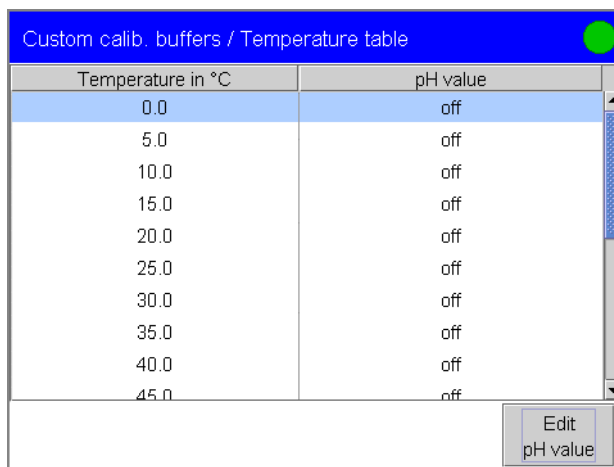
You can define five of your own calibration buffers which can then be used for **calibration with automatic buffer recognition**. The buffer series can be selected in the CAL (calibration) command as the **Custom** buffer series (see Section 4.7).

☞ Open the dialog **Templates/Custom calibration buffers**.



☞ Enter the pH of the first buffer under **Buffer 1**.

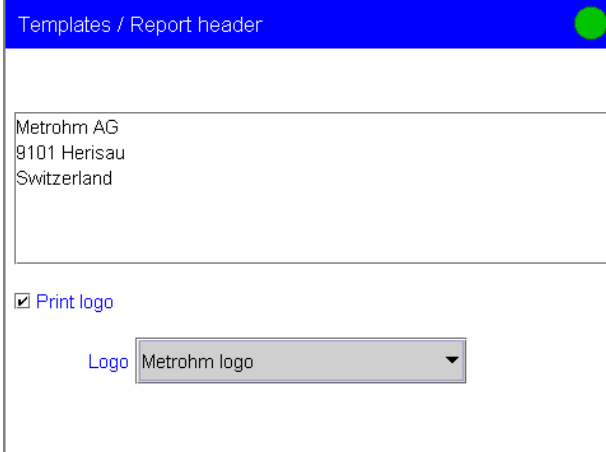
☞ Use **Temp. table** to open the temperature table for this buffer. The temperature table shows the pH values for the buffer at temperatures from 0 to 95 °C.



☞ Use **[Edit pH value]** to enter the pH values for the temperature range in which you perform your pH calibration and pH measurement. In the dialog **[Temperature table/Edit pH value]** you can change directly to the next temperature. If you do not know the pH values for individual temperatures, these will be calculated automatically by linear interpolation.


3.14.7 Report header

You can enter a text here (max. four lines each with 46 characters) which will always be printed out in front of the standard report header (see *Section 3.23*).



☞ Enter the text for your **Report header**. If you want to print out the Metrohm logo to the right of the text then activate the **Print logo** checkbox and select **Metrohm logo** in the selection list. If you wish to print your own logo in the report header select **Custom logo**. The creation of your own logo is described below.

The settings shown above will produce a report header which looks like this:

Metrohm AG 9101 Herisau Switzerland	
PC Control PC Control	Serial number 3079972211 Printed
	Program version 4.1 2006-05-22 16:15:21

Creating your own logo

This is done by using the file **CustomBitmap.gif** in the installation folder of the PC Control Software.

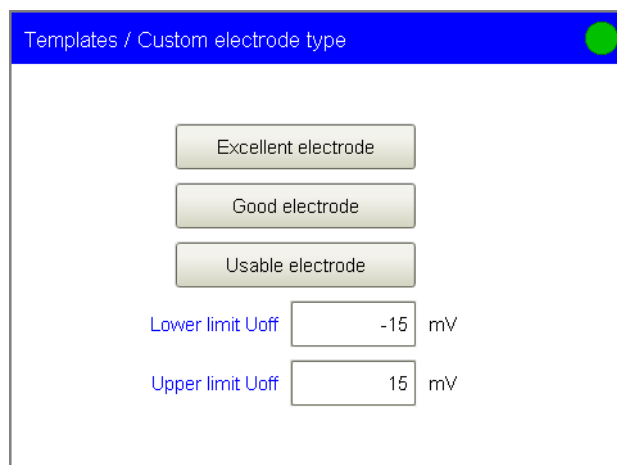
- ☞ Open this file in an image processing program and copy your logo into it. The image must not exceed a size of 472 x 92 pixels. If necessary you must reduce the size of your logo accordingly.
- ☞ Save the image as a gif file.
- ☞ Now select **Custom logo** in the selection list.
- ☞ Under **File/Custom Logo**, enter the path under which you have stored the logo.
- ☞ Activate the option PC Control or Touch Control, depending on what you want to use your logo with. For Touch Control the image is reduced to the eight basic colors red, green, blue, cyan, magenta, yellow, white and black.

- ☞ Confirm with **[Generate]**. In PC Control the logo can be used directly; for Touch Control the file **CustomImage.bin** is generated in Card 1 (see menu Preferences).
- ☞ Save this file onto a memory card, insert it in Touch Control card slot 1 and load the file.
- ☞ This is done by selecting the Touch Control under **Device** in the menu **System/Diagnosis/Software update**. In the selection list **Update Type**, select the item **System file** and confirm with **[Continue]**.
- ☞ Under **Binary file**, open the list with the files on the memory card.
- ☞ Select the file CustomImage.bin with **[Select]** and confirm with **[Continue]**.
- ☞ Press **[Install]**. The file is installed.

3.14.8 Custom electrode type

You can define your own values for the electrode test of pH electrodes instead of the stored limit values. This may be helpful for special applications if, for example, other quality requirements are placed on the pH electrode or work is carried out with a reference electrode which displaces the offset potential U_{off} beyond the required -15 to $+15$ mV (standard and gel electrodes).

- ☞ Open the dialog **Templates/Custom electrode type**.



The limit values can be defined for the following electrode ratings:

- Excellent electrode
 - Good electrode
 - Usable electrode
 - **Lower limit Uoff**: Lower limit for the offset potential, i.e. the potential at $pH = 7.0$. The value applies for all ratings.
 - **Upper limit Uoff**: Upper limit for the offset potential, i.e. the potential at $pH = 7.0$. The value applies for all ratings.
- ☞ Enter the desired values for **Lower/Upper limit Uoff**.
 - ☞ Select an electrode rating.

Custom electrode type / Excellent electrode

Streaming potential	<input type="text" value="2.5"/>	mV
Drift	<input type="text" value="2.0"/>	mV/s
Slope min.	<input type="text" value="96.5"/>	%
Slope max.	<input type="text" value="101.0"/>	%
Response time	<input type="text" value="45"/>	s

- **Streaming potential:** The streaming potential is the difference between the voltages measured in stirred and unstirred solution.
- **Drift:** For each buffer, the drift in stirred solution is determined. The sum of these values is compared with this value here.
- **Slope min.:** Minimum slope of the pH electrode.
- **Slope max.:** Maximum slope of the pH electrode.
- **Response time:** The voltage measured in stirred solution after three minutes serves as a reference value for the determination of the response time. The response time is defined as the time after which the measured voltage is within ± 1 mV of this reference value.

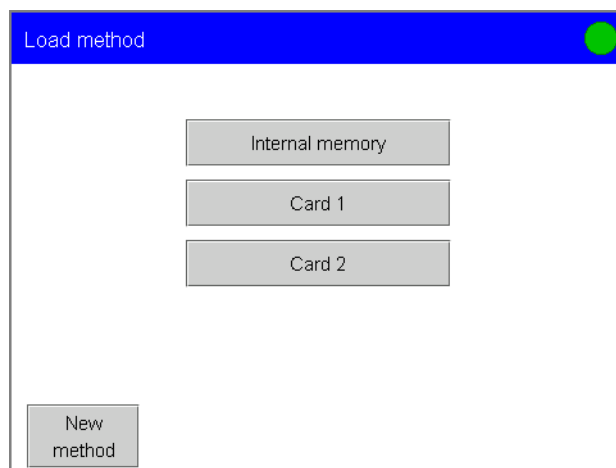
3.15 Loading methods

The sequence of a determination is defined in the **method**. In the **Load method** dialog you can load saved methods or **method templates** for creating new methods.

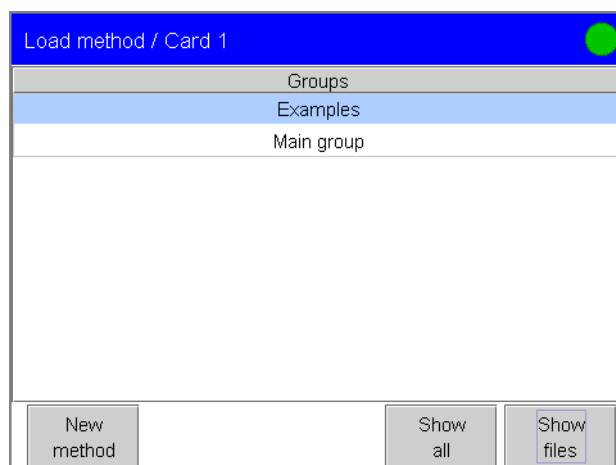
3.15.1 Loading a method

Methods can be saved in the internal memory, on Card 1 or Card 2 or a shared file system (requires 847 USB Lab Link, see *Section 3.10.11*). In a new system no methods are stored in the internal memory which is why the following example describes **loading a method from Card 1**, on which the methods provided as examples are stored.

- ☞ With **Touch Control** insert the supplied data card containing the examples of methods in Card slot 1.
- ☞ From the main dialog open the dialog **Load method** and select **[Card 1]**.

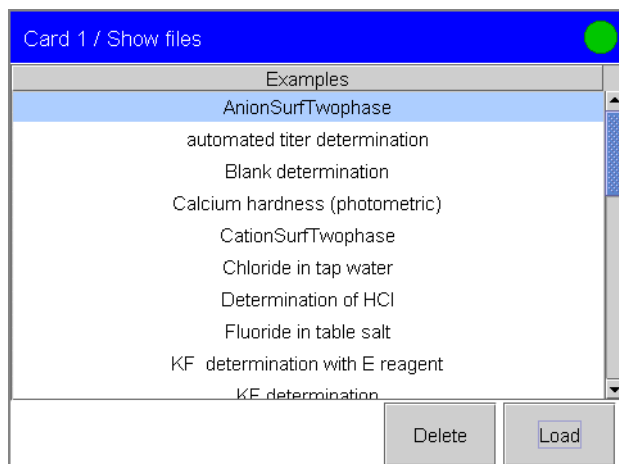


The selection of the memory location will be skipped if only the internal memory is accessible. If several **file groups** exist on the card then a list showing the existing **groups** will be displayed:



The selection of the group will be skipped if only one group is present in the selected memory.

- ☞ Select the group **Examples** and open the file list for this group with **[Show files]**. With **[Show all]** you can open the list of files containing all the methods in the selected memory.



- ☞ Select a method from the list, e. g. **Determination of HCl** and **[Load]** it. When the file has been loaded the program will jump automatically to the main dialog. If the method contains a **Note** which is displayed when the method is loaded then this can be closed with **[Continue]**. You can edit the method with **[Edit parameters]** (see Section 3.16).



Note!

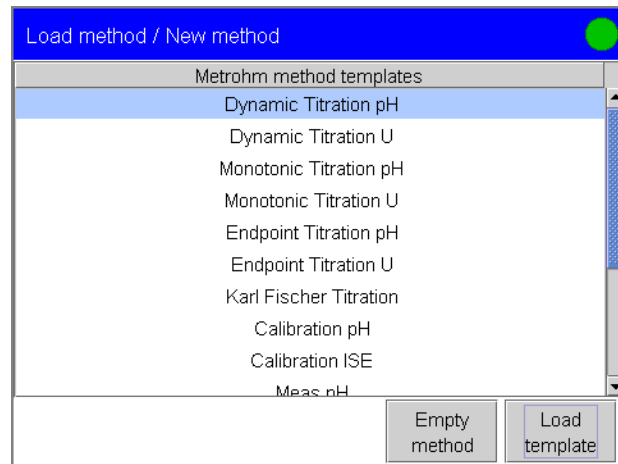
The data of the current **determination** will be **deleted** if a new method is loaded.

You can use the procedure described above to load methods from all available memory locations. The selected file can be removed from the list of files with **[Delete]**. If you have activated **Write protection** for the method in the **File manager** under **Show files/Properties** then it cannot be deleted.

3.15.2 Creating a new method

If you wish to create a new method then you can either load a **method template** from the selection list and adapt it to meet your requirements or load an **"empty" method** in which no sequence of commands has yet been defined.

- ☞ From the main dialog open the dialog **Load method** and then open the list of method templates with **[New method]**.



The individual templates are described on the following pages. The commands in the method templates have standard parameters. These standard parameters are suitable for most titrations.



Note!

*If you would like to test a **new titration method** then select the **Dynamic titration pH or U template**. Dynamic titration is suitable for practically all standard applications and you only have to adapt individual parameters in special cases.*

No results have been defined yet in the calculations (see *Section 4.5.1*).

☞ Select a method template from the list and load it with **[Load template]** or load a method template in which no sequence of commands has yet been defined with **[Empty method]**. When the file has been loaded the program will jump automatically to the main dialog. You can edit the method with **[Edit parameters]** (see *Section 3.16*). This method has the name **New method**. You can change this name when you save the method (see *Section 3.16.11*).

The following **method templates** can be selected:

<i>Method template</i>	<i>Command sequence</i>	<i>Application</i>
Dynamic Titration pH	DET pH (dynamic titration) CALC REPORT (result report and titration curve)	Dynamic reagent addition , for rapid equivalence point titrations, large volume increments in the flat part of the curve; small increments near the EP, many measuring points near the EP. For all standard titrations (acid/base titrations, precipitation titrations, redox titrations).
Dynamic Titration U	DET U (dynamic titration) CALC REPORT (result report and titration curve)	
Monotonic Titration pH	MET pH (monotonic titration) CALC REPORT (result report and titration curve)	Reagent addition with constant volume increments , relatively few measuring points near the EP. For titrations with relatively high signal variations or a suddenly occurring potential jump, very flat potential jumps, slow titrations (non-aqueous titrations, certain redox titrations, surfactant determinations).
Monotonic Titration U	MET U (monotonic titration) CALC REPORT (result report and titration curve)	
Endpoint Titration pH	SET pH (endpoint titration) CALC REPORT (result report and titration curve)	Titration to a predefined endpoint . For rapid routine determinations , titration to particular standards and titrations in which an excess of titrant must be avoided (p+m values, pH adjustment).
Endpoint Titration U	SET U (endpoint titration) CALC REPORT (result report and titration curve)	
Karl Fischer Titration	WAIT REQUEST (data scanning) KFT Ipol (Karl Fischer titration) CALC REPORT (result report and titration curve)	Titration for water determination by Karl Fischer with pre-and post-conditioning.
STAT pH without pre-titration	STAT pH (Titration with holding the measured value constant) EVAL RATE (Rate evaluation) CALC REPORT (result report and titration curve)	Titration to a predefined control point . The control point is kept constant by continuous reagent addition, e. g. for determination of enzyme activity .

<i>Method template</i>	<i>Command sequence</i>	<i>Application</i>
STAT pH with pretitration	SET pH (endpoint titration) WAIT STAT pH (Titration with holding the measured value constant) EVAL RATE (Rate evaluation) CALC REPORT (result report and titration curve)	Titration to a predefined control point . The control point is kept constant by continuous reagent addition, e. g. for determination of enzyme activity .
Calibration pH	CAL pH (calibration of a pH electrode) REPORT (result report with calibration data and titration curve)	Calibration of pH electrodes.
Calibration ISE	CAL Conc (calibration of an ISE sensor) REPORT (result report with calibration data and titration curve)	Calibration of ion-sensitive electrodes.
Meas pH	MEAS pH (pH measurement) CALC REPORT (result report and measurement curve)	pH measurement.
Meas U	MEAS U (potential measurement) CALC REPORT (result report and measurement curve)	Potential measurement.
Meas T	MEAS T (Temperature measurement) CALC REPORT (result report and measurement curve)	Temperature measurement with a temperature sensor (Pt1000 or NTC).
Meas concentration	MEAS Conc (concentration measurement) CALC REPORT (result report and measurement curve)	Ion concentration measurement with an ion-sensitive electrode.

<i>Method template</i>	<i>Command sequence</i>	<i>Application</i>
SP Method rinse sample beaker	MOVE (rotate rack) LIFT (move lift to work position) STIR WAIT STIR SUBSEQ (aspirate and rinse in sample beaker) SUBSEQ (End sequence)	Titration with the USB Sample Processor . The WAIT command must be deleted and replaced by a titration, a CALC and a REPORT command.
SP Calibration and measure	SUBSEQ (Start sequence for pH calibration) SUBSEQ (rinse and aspirate) MOVE LIFT STIR MEAS pH (pH measurement) STIR CALC REPORT (result report) SUBSEQ (End sequence)	pH calibration with subsequent pH measurement with the USB Sample Processor .
SP Pipetting Ext. Position	SUBSEQ (Start sequence) SUBSEQ (pipetting at ext. position) WAIT STIR PUMP SUBSEQ (End sequence)	Pipetting the sample into a beaker at external position 1. The WAIT command must be deleted and replaced by a titration, a CALC and a REPORT command.

**Note!**

If you have no **printer** connected to your system then you should delete all **REPORT commands** from the list of commands.

3.16 Editing parameters

Here you can define and edit the **method commands** which are processed successively during a **determination**.

☞ From the main dialog use **[Edit parameters]** to open the **list of commands** for the current method. If you have loaded a method (see *Section 3.15.1*) then the list of commands will already contain a sequence of method commands. If you have used **[Empty method]** to create a new method (see *Section 3.15.2*) then the list of commands will still be empty.

Parameters / Sequence		
Current method: New method		
01	REQUEST	Data request
02	DET pH	Dynamic pH titration
03	CALC	Calculation
04	REPORT	Report
05	...	
<div style="display: flex; justify-content: space-around; margin-top: 10px;"> Save method Method options Insert command Delete command Edit command </div>		

In the **list of commands** the **command number**, **command name** and the **command comment**, which you can edit yourself, are shown for each command. The last command line is always empty. It can neither be deleted nor edited.

With **[Insert command]** you can insert a new method command in the list in front of the selected command (see *Section 3.16.2*). With **[Delete command]** the selected command is removed from the list. You can edit the parameters for the selected command with **[Edit command]** (see *Section 3.16.1*).

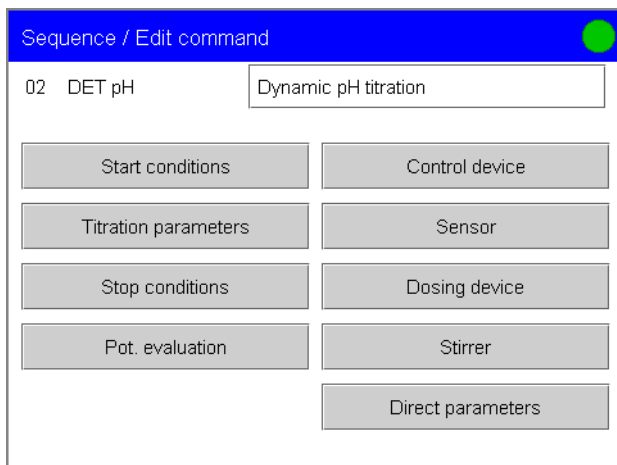
In the dialog **Sequence/Method options** you can make settings which apply to the whole method and not just to individual commands. With **[Save method]** you can store the method in one of the memories (internal memory, Card 1, Card 2, Shared memory) (see also *Section 3.11* and *Section 3.16.11*).

3.16.1 Editing commands

The edit dialog differs greatly according to the number of **parameters** which can be edited in a method command. For example, the REQUEST command requires only a single dialog level for parameter input. Editing a titration (e. g. DET pH) is considerably more complex, although standard titrations can be carried out with the standard parameters and parameters only need to be altered for special applications or instrument configurations. In a CALC command up to nine results can be defined; a calculation formula is entered for each result and various options are defined (see *Section 4.5.1*). An **overview of all**

commands and parameters can be found in *Section 4*. The **input range** for all parameters can be found in the **online help**.

- ☞ Select the command in the list for which you want to edit the parameters and open the edit dialog with **[Edit command]**. In the example shown the command **DET pH** has been selected.



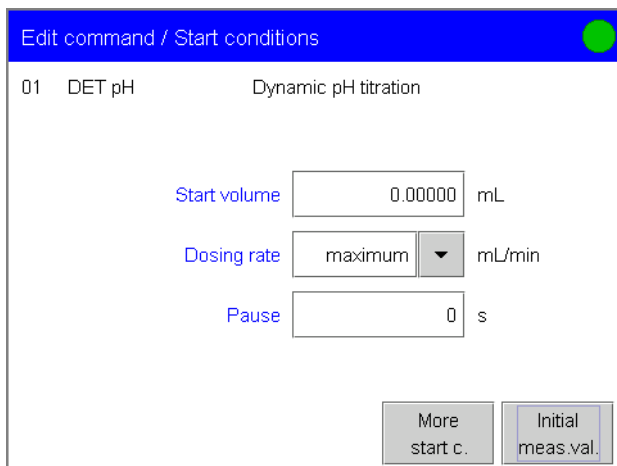
The command number, the command name and the command comment are always shown in the first row. The comment can be edited in the input field.



Note!

The button **Control device** will only be shown when several control devices have been configured in the device manager.

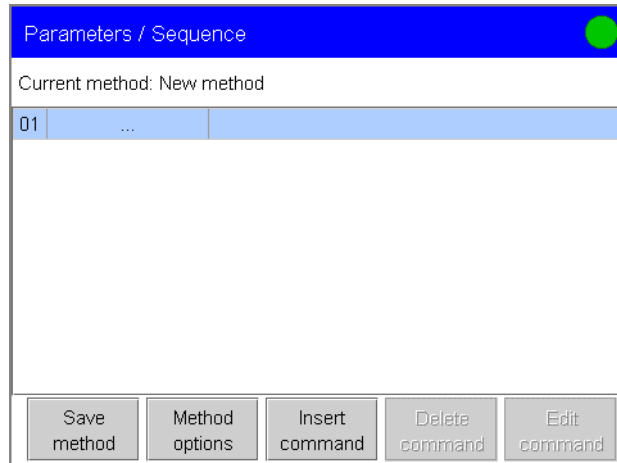
- ☞ Open the edit dialog for the start conditions with **[Start conditions]**.



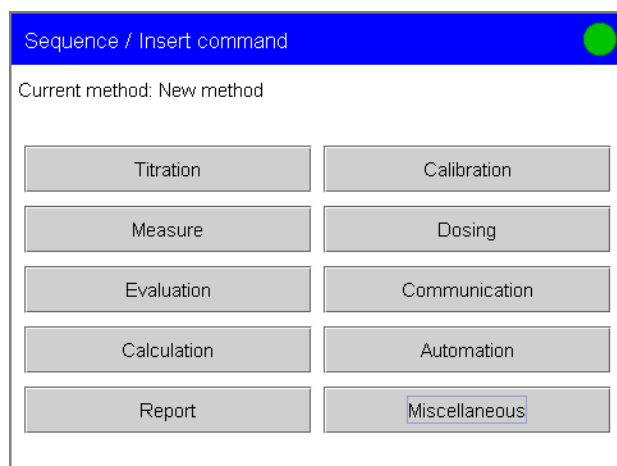
For many parameters (e. g. **Start volume** and **Pause**) you can enter a numerical value directly, with other parameters (e. g. **Dosing rate**) you can use the arrow to the right of the input field to alternatively select a "**special value**" from the selection list. It is often only possible to choose between various settings in a list (e. g. **Measuring input** under **Edit command/Sensor**).

3.16.2 Insert command

A method may contain a max. of 99 commands. You can use **[Insert command]** to insert a new method command in front of the selected line. In the example shown a new "empty" method is being edited.



☞ Use **[Insert command]** to open the dialog **Sequence/Insert command**.



The method commands are arranged in different groups. An **overview of all commands and parameters** can be found in *Section 4*. The individual commands are also described in the **online help**.

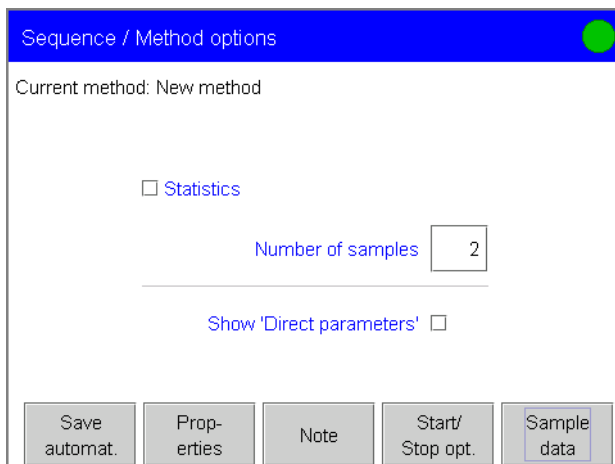
☞ Select the group from which you wish to insert a command. For **Report** the command is inserted directly. For all other groups the command selection list is opened for you to select a command.

After a command has been inserted the list of commands is automatically shown again. The inserted command is shown as selected so that you can use **[Edit command]** directly to edit the parameters of the newly inserted command (see *Section 3.16.1*). You can insert a maximum of nine titrations or measurements and nine calculations. There is no limit to the number of other commands (up to 99 in one method).

3.16.3 Method options

Method options are settings which apply to the method as a whole and not to an individual command. For example, you can switch **Statistics** on and off, **Show direct parameters** on and off, **automatically save the determination at the end of the run**, **sign a method**, enter a **Note** and make the **settings for sample data input**.

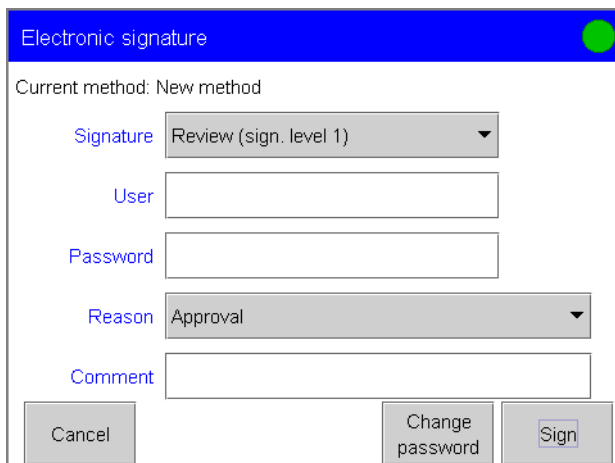
☞ Open the dialog **Sequence/Method options**.



[Properties] accesses an overview of the properties of the current method. If you are not working with login and password or if the method has never been saved then the buttons **[Delete signature]** and **[Sign]** will be inactive. The button **[Delete signature]** is inactive for as long as the method has not been signed at level 2. If the method has been signed three times at level 2 then the only active button is **[Delete signatures]**.

[Sign] accesses the dialog for signing methods.

Sign



- **Signature:** Selects the level at which the method should be signed. If the method has never been signed then only level 1 can be selected. If the method has been signed three times at level 1 or already once at level 2 then only level 2 can be selected. A maximum of three signatures from up to three different users can be given at each level. However, it is not possible for a user to sign at both level 1 and level 2.

- **User:** Enters the identification of the user who signs. In the overview of the method properties the name of the user appears as given under **User admin./Edit** under **Full name**. If no complete name has been entered there then the identification appears in the overview of the method properties.
- **Password:** Enters the password.
- **Reason:** Selects the reason for the signature. Under **Login options/Reasons** (see *Section 3.7.7*) the list of reasons can be defined by users with Administrator rights.
- **Note:** A note in addition to the reason can be entered here.

[Cancel] rejects the entries and returns to the overview of the method properties. You can also **[Change password]** here. With **[Sign]** the method with the given data is signed and a return is made to the overview of the method properties.

Only saved methods can be signed. The current status of a method can be seen under **Method options/Properties**. An overview of the possible method statuses can be found in the **Online help** for the dialog mentioned. If under **Login options/Modification options** (see *Section 3.7.7*) you have defined that a reason is to be demanded for method modifications then this reason will only be demanded when the method has the status **"modified"**. If a saved method has been altered but not yet resaved then its status is **"modified"**.

Delete signature

If a released method has to be revised, e. g. for adaptation to changed conditions, the signatures must be deleted before the method sequence can be edited. However, signatures can only be deleted when the method has been signed at level 2. If the method has been signed at level 1 then the signatures will be deleted automatically as soon as the method is modified.

- **User:** Identification of the user who deletes the signatures.
- **Password:** Enters the password.
- **Reason:** Selects the reason for the deletion of the signatures. Under **Login options/Reasons** (see *Section 3.7.7*) the list containing the reasons can be defined by users with Administrator rights.
- **Comment:** A comment in addition to the reason can be entered here.

[Cancel] rejects the entries and returns to the overview of the method properties. **[Delete signature]** deletes all the signatures to the method and returns to the overview of the method properties. The method then has the status "**Saved**".

3.16.4 Statistics

If you want to statistically evaluate certain **results**, which have been calculated during the determination sequence then you must make the following settings:

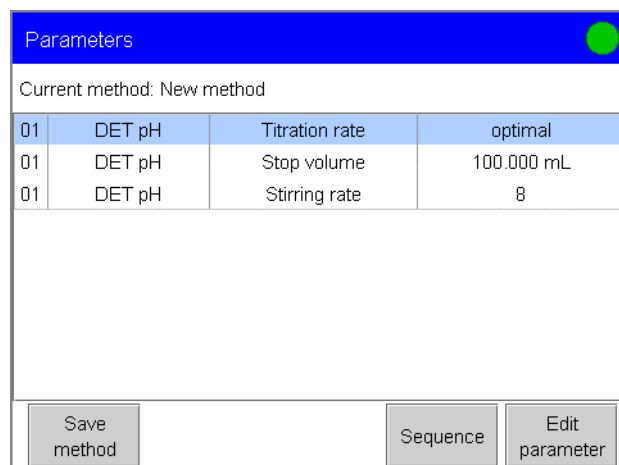
- ☞ Activate the **Statistics** checkbox.
- ☞ Enter the **Number of samples** on which the statistics are to be based. For example, if you carry out a three-fold determination then you should enter **3**.

The results for which statistical calculations are to be carried out are defined in the **CALC command** (calculation).

3.16.5 Direct parameters

Direct parameters can be defined for many method commands; they are then shown in a table when the parameter dialog is opened and can be edited directly. The direct access ("**Quick Access**") to the edit dialog for selected method parameters simplifies the editing of parameters which need to be changed frequently.

- ☞ Activate the **Show direct parameters** checkbox and use **[Home]** to return to the main dialog. Now open the **Direct parameter list** with **[Edit parameter]**.



The screenshot shows a dialog box titled "Parameters" with a blue header and a green close button. Below the header, it says "Current method: New method". A table lists three parameters for a DET pH titration:

01	DET pH	Titration rate	optimal
01	DET pH	Stop volume	100.000 mL
01	DET pH	Stirring rate	8

At the bottom of the dialog, there are three buttons: "Save method", "Sequence", and "Edit parameter".

The above example shows the direct parameters for a DET pH titration with standard settings. The parameters that are to be shown in the direct parameter list can be selected for each command in which direct parameters are available (see *Section 4*) under **Edit command/Direct parameters**.

You can open the edit dialog for the selected command with **[Edit parameter]** and then edit the parameter. The **command list** is opened with **[Sequence]**. **[Save method]** is used to store the method in one of the file memories (internal memory, Card 1, Card 2, Shared memory) (see also *Section 3.11* and *Section 3.16.11*).

3.16.6 Sample data

In the method you can adapt the **label of the sample identifications** 1 and 2 which are shown in the main dialog. You can also define the **Sample size unit** or a **Fixed sample size**. The sample size can then no longer be edited in the main dialog. If you define **Sample size limits** then these will be monitored during the determination after START and at the end of the determination.

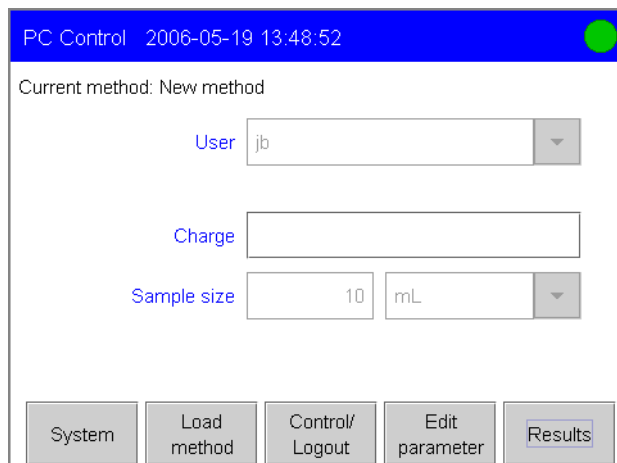
If you do **not want to show an identification** in the main dialog you can deactivate the checkbox for the corresponding identification. If you want to enter different method-independent labels for the identifications, e. g. batch number, density, etc. then you can enter your own labels under **Label**. These will be updated in the main dialog and when the sample data is requested with a REQUEST command.

For the **Sample size** you can either enter a **unit** or select one; this will be shown in the main dialog but can still be altered later. The unit will be updated each time that the method is loaded in the main dialog.

If you always use the same amount of sample for your determinations then you can define a **Fixed sample size** in the method. The sample size is shown in the main dialog and can no longer be edited.

☞ Enter, for example, "Charge" as label for **Identification 1** and deactivate the checkbox for showing **Identification 2**. Activate the **Fixed sample size** checkbox and enter "10 mL" as the **Sample size**. Use **[Home]** to return to the main dialog.

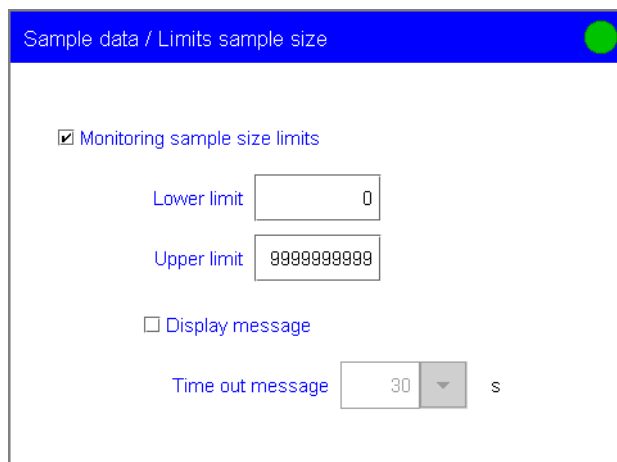
The main dialog will now appear as shown below:



Only Identification 1 is shown with the title "Charge". The fixed sample size "10 mL" is shown and cannot be edited.

You can also define the **limits for the sample size** which will then be monitored in the determination sequence.

☞ Open the dialog **Sample data/Sample size limits** and activate the **Monitoring sample size limits** checkbox.



☞ Enter a **Lower limit** and an **Upper limit** for the sample size.

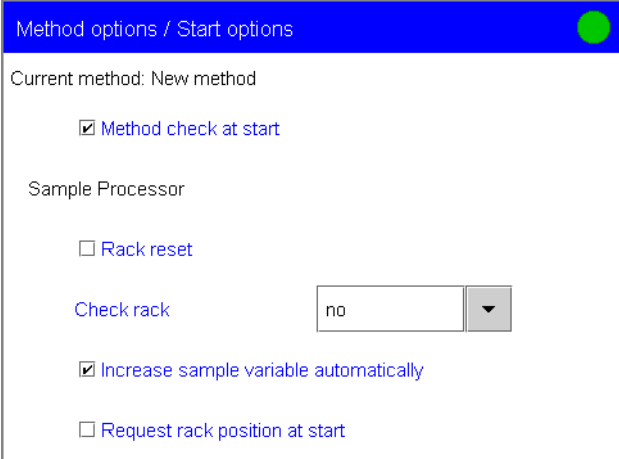
The limits will not be monitored when the sample size is entered in the main dialog, but at the START of the determination and at its end, when an automatic sample data request is made with a REQUEST command and on recalculating a determination. It does not matter whether the sample size has been entered in the main dialog "by hand", transmitted by a balance or barcode reader or entered in the sample data silo. When monitoring is switched on and the limits for the sample size are infringed then an **entry in the message list** for the determination will be made automatically (see *Section 3.18.2*).

Activate the **Display message** checkbox if a message is to be shown during a determination sequence to indicate that the sample size limits have been infringed. You then have the choice of continuing the run or of canceling it. This **Message** can be provided with a **Time out**, i.e. it will vanish automatically when the given time has elapsed and the run will be continued automatically.

3.16.7 Start and stop options

Under **Method options/Start/Stop options** you can switch various start and stop options on and off.

Under [**Start options**] you can switch off the **Method check**, which is carried out automatically after the START of a determination. This avoids delays after the START. The Method check verifies whether all devices, titrants and sensors which are necessary for the run are present and whether monitoring intervals for the titrants and sensors used have expired.



Method options / Start options

Current method: New method

Method check at start

Sample Processor

Rack reset

Check rack ▼

Increase sample variable automatically

Request rack position at start

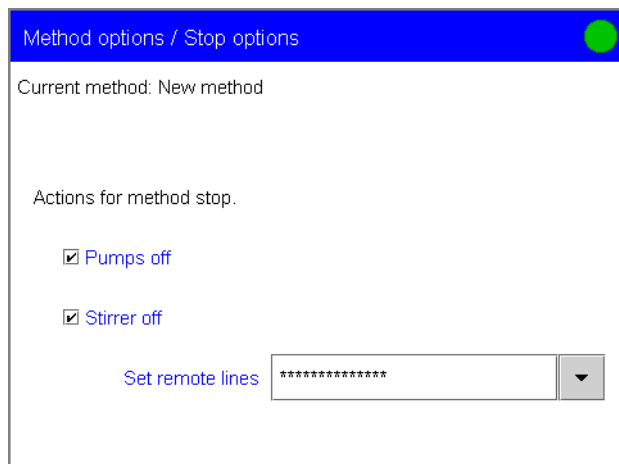
**Note!**

We recommend that you only switch **Method check** off when the titration must be started directly after the START of the determination. For example, this is the case with **very rapid reactions** such as enzyme-catalyzed reactions. Otherwise the determination sequence could be interrupted because e. g. devices, titrants or sensors are not present and available for the determination. Even if the Method check is switched off then the monitoring intervals for titrants and sensors will be checked during the run anyway.

If a USB Sample Processor is used then you can choose whether the **rack** is to be **reset** (see Section 4.12.4) at the start of a method or not. With **Check rack** you can select a rack that must be present when the rack is reset. If a different rack is found then a corresponding error message will be produced. In this way you can make sure that a method is only carried out with this particular rack. If the sample variable at the end of a determination is not to be automatically increased by the value 1 then you can switch off the function **Increase sample variable automatically**. This is important if, for example, you want to selectively influence the sample variable by using the SAMPLE command (see Section 4.12.5). If the rack position of the first sample should be requested at the start of the method then activate the parameter **Request rack position at start**.

Under [**Stop options**] you can switch the actions on and off that are to be taken when a method is stopped. A method can be stopped in the following ways:

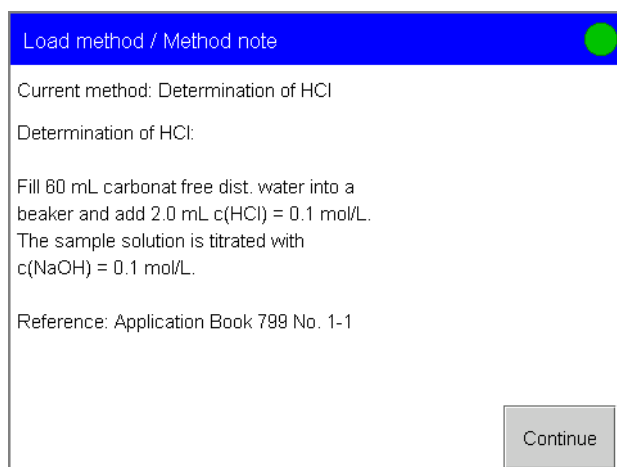
- Manual termination with the **[STOP]** fixed key
- Termination because of an error
- Termination by remote signal via the Control remote box



If the checkboxes **Pumps off** and **Stirrer off** are activated then, when a method is stopped, all the connected pumps and stirrers will be switched off. Under **Set remote lines** you can enter a binary pattern or select a signal from the templates. The templates are defined under **System/Templates/Output lines**. For entering a binary pattern please consult the Online help.

3.16.8 Note

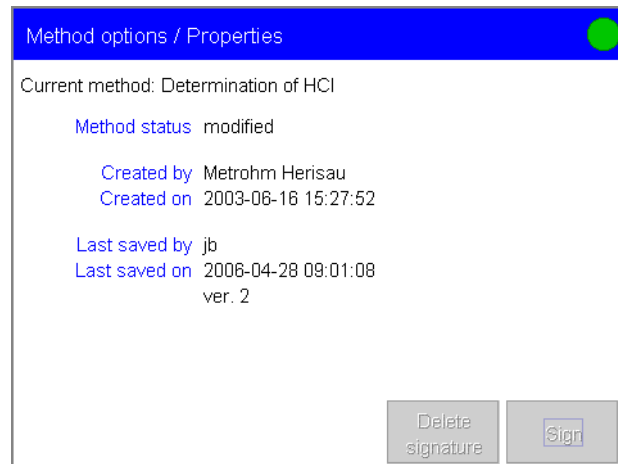
Under **Method options/Note** you can enter a short description of the method. If you activate the **Automatically after loading the method** checkbox under **Note/Display options** then the note will be shown after the method has been loaded. The note is concluded with **[Continue]**. You can exit the note dialog with **[Back]** or **[Home]**. You can use this function to provide the user with further important information about carrying out the determination. For example, after loading the method example **Determination of HCl** the following note will be displayed:



This function should not be used when the method is loaded automatically when processing a sample data silo (see *Section 3.19.3*).

3.16.9 Properties

The properties of the current method are shown under **Method options/Properties**.



An explanation for the individual entries can be found in the **online help**. The method shown as the example has already been saved twice (**version 2**). In comparison to the stored version 2 further parameters have been edited, so that the **Method status** is not **saved** but **modified**.

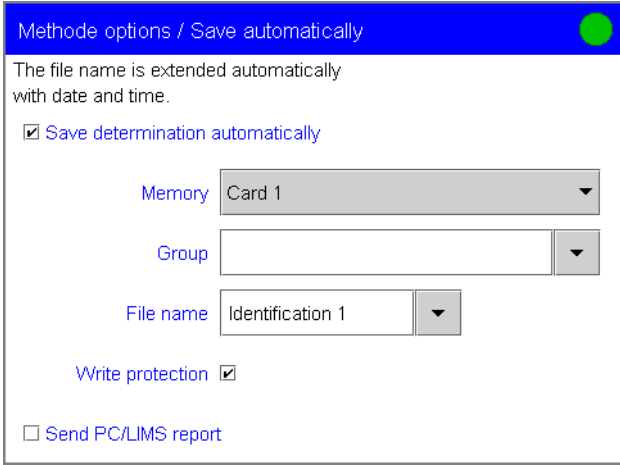
Information about the first person to save the method and when it was first saved (**Created by** and **Created on**) is given together with the last person to save the method and when it was last saved (**Last saved by** and **Last saved on**). Each time that the method is saved under the same name the version number is increased by one, even when the method is saved in a different memory.

If under **Login options/Modification options** the entry of a reason for altering methods is activated then the user who altered the method will be given together with the exact time at which the alteration was made and the reason for it. If the method has been signed then the person who signed will also be documented automatically together with when and at what level (**Reviewed/Released by** and **Reviewed/Released on**) the method was signed.

3.16.10 Saving the determination automat. and sending a PC/LIMS report

In the method you can define that the **determination data** is to be saved automatically at the end of the determination sequence and/or saved or transmitted as a **PC/LIMS report**.

☞ Open the dialog **Method options/Save automatically** and activate the **Save determination automatically** checkbox.



Methode options / Save automatically

The file name is extended automatically with date and time.

Save determination automatically

Memory Card 1

Group

File name Identification 1

Write protection

Send PC/LIMS report

☞ Under **Memory** select the memory location in which the determinations are to be stored. Determinations can only be stored on **Card 1** or **Card 2** or a shared file system (requires 847 USB Lab Link, see *Section 3.10.11*). Enter the **Group** in which the determinations are to be stored.

If you have retained the standard settings for the **File name** then it will be made up of the first 16 characters which you have entered for **Identification 1** and the **determination time** (date and time): Identification 1-YYYYMMDD-hhmmss. For the first 16 characters of the file name you can also select **Identification 2** or **the name of the method** or you can enter a different text. The date and time will be appended so that the file name is always unambiguous.

If the **Write protection** checkbox is activated then the saved determination files will be automatically write-protected and therefore protected against accidental alterations or alterations by unauthorized persons. This function is switched on by default so that the **original data** is also retained.

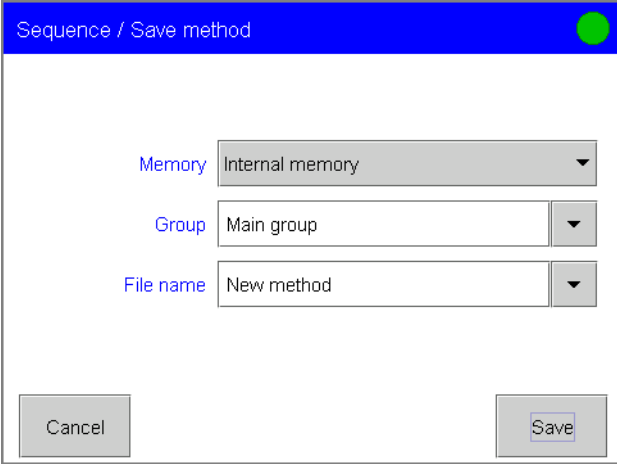
If the **Send PC/LIMS report** checkbox is activated then an ASCII report containing all the important data of the determination will be sent automatically at the end of the determination. The settings for sending and saving the PC/LIMS report are made in the device manager under **Edit device/PC/LIMS report** (see *Section 3.10.12*). The file name corresponds to the name of the determination preceded with PC_LIMS_Report-. I.e. the format is PC_LIMS_Report-Identification 1-YYYYMMDD-hhmmss.txt if you keep the default settings for the **File name** under **Save determination automatically**. The date and time correspond to the determination time. A detailed description of the contents of the PC/LIMS report can be found in the Titrando **PC/LIMS Report Guide**.

3.16.11 Save method

You can save the current method in one of three memories (see *Section 3.11*).

- ☞ From the main dialog use **[Edit parameter]** to open the **command list** for the current method. If the use of direct parameters has been switched on (see *Section 3.16.5*) then the **direct parameter list** will be opened; the method can also be saved from here.
- ☞ Use **[Save method]** to open the dialog for selecting the memory, file group and file name.

If you have created a new method (see *Section 3.15.2*) and this has still not been saved then the dialog **Sequence/Save method** will look like this:



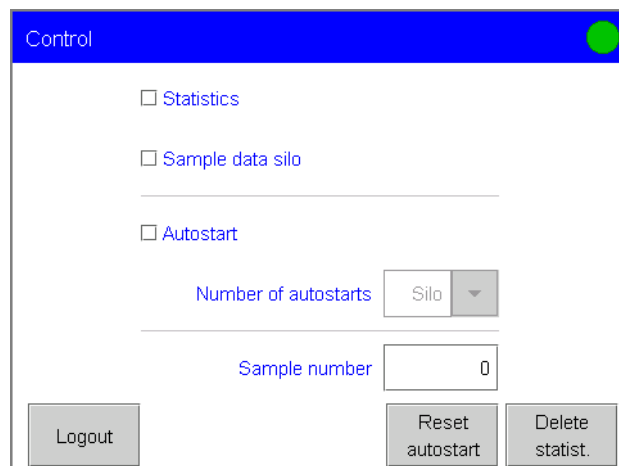
The screenshot shows a dialog box titled "Sequence / Save method". It features three dropdown menus for selection: "Memory" (set to "Internal memory"), "Group" (set to "Main group"), and "File name" (set to "New method"). At the bottom of the dialog, there are two buttons: "Cancel" on the left and "Save" on the right.

- ☞ Under **Memory** select the memory location in which the method is to be saved. Methods can be saved in the **Internal memory**, on **Card 1** or **Card 2** or a shared file system (requires 847 USB Lab Link, see *Section 3.10.11*).
- ☞ In order to arrange your methods they can be stored in different groups. Enter the **Group** in which the method is to be saved. You can also select the group from the list of existing file groups. If the method has already been stored then the group in which the method has already been stored will be proposed. The **file names** must be **unambiguous** for each memory location, i.e. you cannot save a file in different groups with the same name.
- ☞ Enter a **File name** for the method. If the method has already been stored then the name under which the method has already been saved will be proposed. The method is saved with **[Save]**. With **[Cancel]** and **[Back]** the method is not saved.

3.17 Control

This is where various **settings** for a determination run or for processing a series of samples are made. If you are working with login (see [Section 3.7.7](#)), then you can use **[Logout]** in this dialog to log out of the system. The login dialog will then be shown.

☞ From the main dialog open the **Control** dialog.



The **Sample number** is primarily used for documentation. Each time that a determination is started with START it is increased by one. Each time that the system is started (by starting the PC Control software or switching on Touch Control) it is reset to zero. You can also enter a sample number yourself.

3.17.1 Statistics

In the **Control** dialog you can switch **Statistics** on and off for individual determinations. Whether this checkbox is activated when the dialog is opened depends on whether statistics has been activated in the method under **Method options** (see [Section 3.16.4](#)). When a method is loaded the setting under Control is updated automatically.



Note!

*If you activate **Statistics** in the method under **Method options** then **Statistics** under **Control** will be activated automatically.*

This button is chiefly required to enable an "**urgent sample**" to be inserted while a series of samples is being processed without it being included in the statistics calculations. If you process the "urgent sample" with the same method as the sample series then you only have to switch the statistics button off while the urgent sample is being processed and then on again after it has been processed. If the "urgent sample" has to be processed with a different method then proceed as follows:

- ☞ Save the current sample series determination (see [Section 3.18.5](#)) and load the method for the "urgent sample".
- ☞ Carry out the determination for the "urgent sample".

- ☞ Load the last determination in the sample series that you have previously saved (see *Section 3.18.6*). The method used and the current statistics data will also be loaded together with the determination. The statistics button under **Control** and the statistics counter will have the same status as they had before the interruption to the sample series.
- ☞ Continue with the processing of the sample series.

You can view the statistics overview under **Results/Statistics** (see *Section 3.21*). With **[Delete statistics]** you can delete the statistics data manually.

The statistics data is deleted automatically in following cases:

- when the actual statistics counter (number of processed samples) is the same as the preset number of determinations used for the statistics. The maximum value of the statistics counter is defined under **Sequence/Method options**.
- when a method is loaded with **[Load method]**. It does not matter whether this is the same method that was previously loaded. If you use either the sample data silo or the sample assignment table then a check will be made whether the method is the same (file name is the same) as that already loaded. Only when this is a different method will the new method be loaded and the statistics deleted.
- when a determination is loaded. At the same time the method with which the statistics have been calculated is also loaded.

3.17.2 Sample data silo

Under **Control** you can switch on the use of the sample data silo. The **sample data silo** is a table in which the sample data for a sample series can be entered and stored. If you have activated the **Sample data silo** checkbox then at each START of a determination the sample data will be taken from the silo memory. You can then open the sample data table in the main dialog with **[Sample data silo]**. The input of the sample data is described in *Section 3.19.3*.

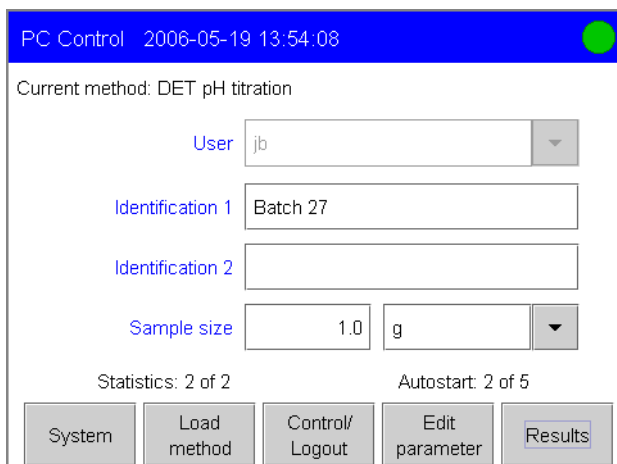
With **[Delete silo]** (Touch Control only) you can delete all the lines in the current silo. The settings made under **Sample data silo/Properties** are retained.

3.17.3 Autostart

The autostart function is used for processing a sample series. If the **Autostart** checkbox is activated then a new determination will be started automatically when a determination has ended until the set **Number of autostarts** has been reached. The number of autostarts can also correspond to the number of samples defined in the sample data silo (see *Section 3.19.3*).

If you deactivate the **Autostart** checkbox while a determination is running then the current determination will be concluded but no new START will take place. With **[Reset Autostart]** you can reset the autostart counter, i.e. the number of autostarts which have already been carried out in a series, to zero.

The current **statistics status** and the current **autostart status** will be shown in the main dialog when these functions have been switched on.



PC Control 2006-05-19 13:54:08

Current method: DET pH titration

User: jb

Identification 1: Batch 27

Identification 2:

Sample size: 1.0 g

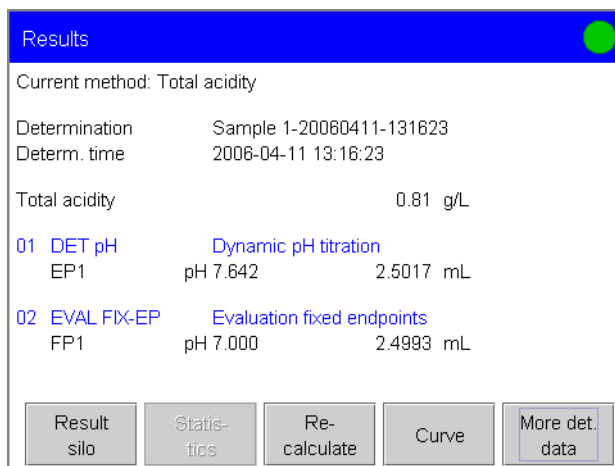
Statistics: 2 of 2 Autostart: 2 of 5

System Load method Control/Logout Edit parameter Results

3.18 Results and more determination data

The most important **details of the current determination** (method used to carry out the determination, name of the determination, determination time), the **calculated results** (result name and result with unit) and the **raw data** (e. g. endpoints or final measured values) are shown under **Results**.

☞ From the main dialog open the **Results** dialog.



You can use **[More determination data]** to view further data about the current determination (list of measuring points, details of the endpoints, messages produced during the determination, properties of the determination, devices used, etc.). Additionally you can **load and save determinations**. For the current determination you can use **[Curve]** to view the titration or measurement curve, etc. and **[Recalculate]** to recalculate and re-evaluate the determination.

If a SIGN command is inserted in the method sequence, the button **[Sign]** is displayed instead of **[Recalculate]** and the determination can be signed at level 1 right at the end of the sequence (signing at level 2 with a second SIGN command). This button is only active if you are working with login and password.

From the results dialog you can also open the **Result silo**, an overview with results that have been stored (see *Section 3.22*), and the **Statistics overview** of a multiple determination (see *Section 3.21*).

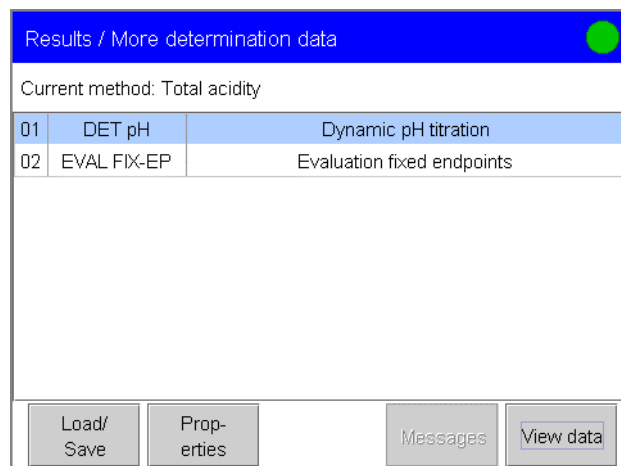
**Note!**

The data of the current **determination** will be **deleted** if a new method is loaded.

3.18.1 More determination data

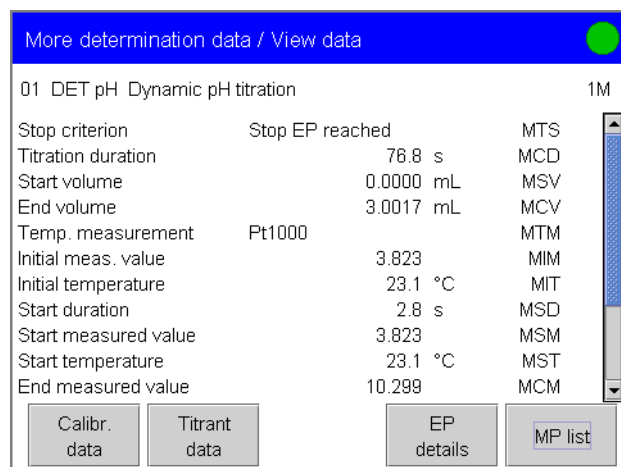
Under **Results/More determination data** a list containing all the method commands which produce raw data (titrations, measurements, calibrations and monitored dosing) and evaluations (EVAL commands) is shown.

☞ Open this list with **[More determination data]**.



Under **View data** the details (**raw data** and **variables**) for the selected command are shown.

☞ Select a command and press **[View data]**.



In the first line the command and the command identification are shown (in the above example **1M**, i.e. the first titration/measurement command). The command identification is used for the unambiguous assignment of the variables to a mode. If only one titration or measurement is carried out in a determination then the command identification does not need to be given.

Below this is a list of raw data and variables. The abbreviation of the variable is shown for variables which can be used in calculations. The individual variables are described in *Section 4.5.7*. In addition to the variables, the **Stop criterion** used to stop the titration, measurement, etc. (manual stop, stop volume reached, error, etc.) and the type of **temperature measurement** (Pt1000, NTC or manual) are shown.

The **[Calibration data]** and **[Titrant data]** buttons are only present when the determination has been loaded. With **[EP details]** you can view details of the endpoints. This button is only available for the titration modes DET, MET, SET and KFT. With **[MP list]** you can open the **list of measuring points** of a titration, measurement or monitored dosing.

List of measuring points

The list of measuring points is displayed in the dialog **View data/MP list**.

☞ Press **[MP list]**. This button is only available for titrations, measurements and monitored dosing.

Volume [mL]	Meas. value [pH]	ERC
0.00000	3.823	0.0
0.01000	3.826	2.9
0.02000	3.829	3.3
0.03000	3.833	3.2
0.18475	3.884	2.9
0.35075	3.939	2.7
0.52800	3.998	2.7
0.70450	4.057	2.8

With the **[Print]** fixed key you can print out the complete list of measuring points.

☞ With **[View]** you can choose the quantities to be shown in the three columns. The quantities that can be selected depend on the mode. The settings are stored separately and system-specifically for each mode.

Endpoint details

Additional data about the equivalence points or endpoints are displayed in the dialog **View data/EP details**.

☞ Press **[EP details]**. This button is only available for the titration modes DET, MET, SET and KFT.

View data / EP details		
01 DET pH Dynamic pH titration		1M
Endpoint 1		
Volume	2.5017 mL	EP1
Measured value	pH 7.642	EM1
ERC	78.8	EF1
Time	53.6 s	ED1
Temperature	23.2 °C	ET1

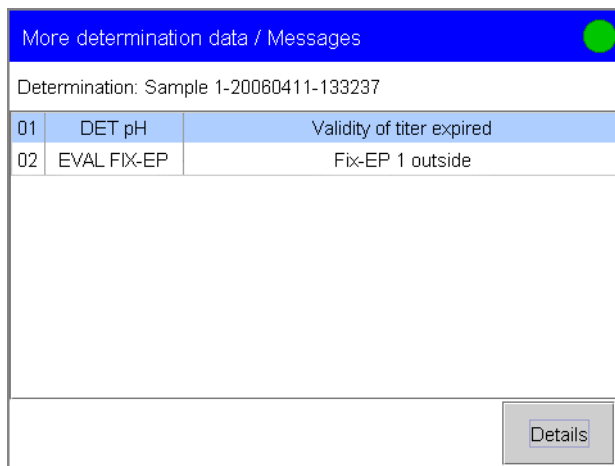
The individual variables are described in *Section 4.5.7*. The **ERC** (**E**quivalence point **R**ecognition **C**riterion) is a measure of the size of the jump in the titration curve. The ERC found is compared with EP criterion defined in the method for the **evaluation of the titration curve** (see *Section 4.1.1*). The ERC is therefore an important quantity if you have to adapt the parameters for the evaluation of the equivalence points.

Calibration and titrant data

The **[Calibration data]** and **[Titrant data]** buttons in the dialog **More determination data/View data** are only present when the determination has been loaded. In these dialogs the sensor data and titrant data that were valid at the time when the determination was carried out are shown. The **concentration** and **titer** of the titrant can be subsequently altered here. When a loaded determination is recalculated (see *Section 3.18.8*), the values shown here are used for the variables TITER and CONC (concentration). Thereby, the values saved under **System/Titrants** are not changed. The **Calibration data** cannot be altered at a later date.

3.18.2 Messages

If **Messages** are produced during a determination sequence then these will be shown under **More determination data/Messages**. The **[Messages]** button in the dialog **Results/ More determination data** is only active when messages have been entered during the run.



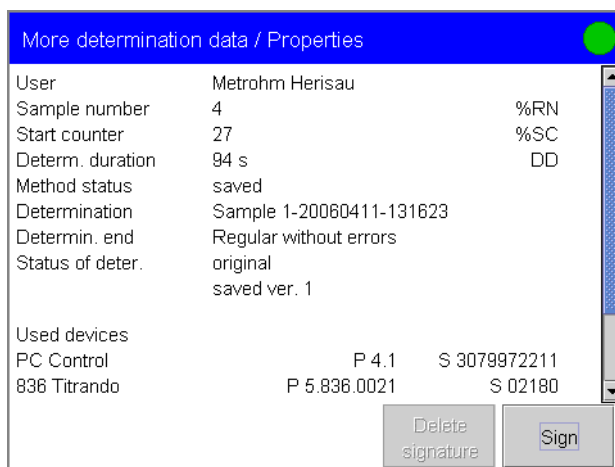
With **[Details]** you can show the unambiguous identification number of the message, the time when the message was produced during the run and the message text for the selected message.

3.18.3 Local common variables

The **[Local common variables]** button in the dialog **Results/More determination data** is only present when the determination has been loaded. In this dialog the list of common variables as they were at the time when the determination was carried out is shown. The common variables can be edited. When a loaded determination is recalculated (see *Section 3.18.8*), the values shown here are used for the common variables CV01 to CV25. Thereby, the list of common variables stored under **System/Common variables** is not altered.

3.18.4 Determination properties

Use **[Properties]** to open the dialog **More determination data/Properties** in the dialog **Results/More determination data**. Various details of the current determination are shown here. The abbreviation of the variable is shown for variables which can be used in calculations. The individual variables are described in *Section 4.4.7*.



The following data is shown for each determination:

- The user who was logged in when the determination was carried out is shown under **User**. If you are working with login and password protection (see *Section 3.7.7*), you can be certain that **only authorized users** can carry out determinations.
- Under **Sample number** the sample number entered at the end of the determination under **Control** is shown.
- The **Start counter** is, like the sample number, increased by one at each START of a determination. However, the start counter cannot be reset by the user. This therefore permits a check of the **uninterrupted documentation of all determinations**. You can see how often the Titrand system has been started from the start counter.
- The **Determination duration** is the time between the START of the determination and the proper end of the sequence or manual termination with **[STOP]**.
- Under **Method status** the status of the method which was used to carry out the determination is shown (see **online help**). The **Method name** is shown under **Results**.
- Under **Determination** the name of the determination will be shown if it has been saved.
- Under **Determination end** the way in which the determination was ended is shown (see **online help**).
- The **Determination status** shows the current status of the determination (see **online help**).

The following information will only be shown if the determination has been recalculated. If under **Login options/Modification options** (see *Section 3.7.7*) the entry of a reason for recalculations has been activated then the reason and any comment accompanying it will be shown.

- **Recalculated by** shows the user who was logged in when the determination was recalculated for the last time.
- **Recalculated on** shows the date and time when the determination was recalculated for the last time.

The following information will only be shown when the determination has been signed at level 1.

- The user who signed the determination at level 1 is shown under **Reviewed by**.
- The date and time at which the determination was signed at level 1 is shown under **Reviewed on**.

The following information will only be shown when the determination has been signed at level 2.

- The user who signed the determination at level 2 is shown under **Released by**.
- The date and time at which the determination was signed at level 2 is shown under **Released on**.

A determination can be signed up to three times at each level.

The **devices** used for the determination sequence are shown for each determination. This means that you can document the devices used to carry out each determination.

- **Touch Control** with program version (P) and serial number (S) or **PC Control** with program version (P) and serial number (S) of the dongle (authorization plug). If no dongle is connected then "Demo version" will be shown.
- Control device (**Titrande** etc.) with program number (P) and serial number (S).
- **Measuring input** with ADC type and serial number.
- The connected devices (dosing device with exchange or dosing unit, stirrer, remote box) with serial numbers are shown for each **MSB** connection (1 to 4).

Sign

If you are working with login and password then the button **[Sign]** is active. **[Delete signature]** is only active if the determination has been signed at level 2.

- **Signature:** Selects the level at which the determination should be signed. If the determination has never been signed then only level 1 can be selected. If the determination has been signed three times at level 1 or once already at level 2 then only level 2 can be selected. A maximum of three signatures from up to three different users can be given at each level. However, it is not possible for a user to sign at both level 1 and level 2.
- **User:** Identification of the user who signs.
- **Password:** Enters the password.
- **Reason:** Selects the reason for the signature. Under **Login options/Reasons** (see *Section 3.7.7*) the list containing the reasons can be defined by users with Administrator rights.
- **Comment:** A note in addition to the reason can be entered here.

[Cancel] rejects the entries and returns to the overview of the determination data. You can also change the password here. With **[Sign]** the determination with the given data is signed and you return to the properties of the determination.

Delete signature

If the determination has already been signed at level 2 then you can delete all signatures with **Delete signature**. If the determination has been signed at level 1 then the signatures will be automatically deleted as soon as the determination is recalculated.

- **User:** Enters the user who deletes the signatures.
- **Password:** Enters the password.
- **Reason:** Selects the reason for the deletion of the signatures. Under **Login options/Reasons** (see *Section 3.7.7*) the list containing the reasons can be defined by users with Administrator rights.
- **Comment:** A note in addition to the reason can be entered here.

[Cancel] rejects the entries and returns to the overview of the determination data. With **[Delete signature]** all the signatures for the

determination are deleted and you return to the properties of the determination.

3.18.5 Save determination

You can save the **current determination** on Card 1, Card 2 or a shared file system (requires 847 USB Lab Link, see *Section 3.10.11*). In this way you can store all the data of a determination. If you wish to save every determination then you can use the function **Save automatically** (see *Section 3.16.10*). Under **Sequence/Method options** you can define that all the determination data is to be saved at the end of each determination. If the data is saved automatically with the standard settings then each determination will be automatically **write-protected**. In this way your original data is protected and can neither be edited nor deleted.

- ☞ In the dialog **Results/More determination data**, open the selection **Load/Save**.
- ☞ Press **Save**. The procedure for saving a file is described in *Section 3.11.4*. The file name **Identification 1-YYYYMMDD-hhmmss** is proposed as default. This means that the file name consists of the text entered as Identification 1 and the determination time. You can also enter any other file name you choose. The extension of the file name with the determination time has the advantage that the file names of all determinations are unambiguous.

The following data is stored for each determination:

- Calculated results.
- All raw data (measuring point lists, endpoints...) and variables produced during the determination.
- Determination properties.
- Statistics, if statistical calculations have been carried out.
- Method with which the determination was carried out.
- Common variables (values and properties of all common variables at the time of the determination).
- Most important titrant data for the titrants used.
- Most important calibration data for the sensors used.



Note!

The data saved with each determination ensures that the data is traceable and that the documentation is GLP-conform.

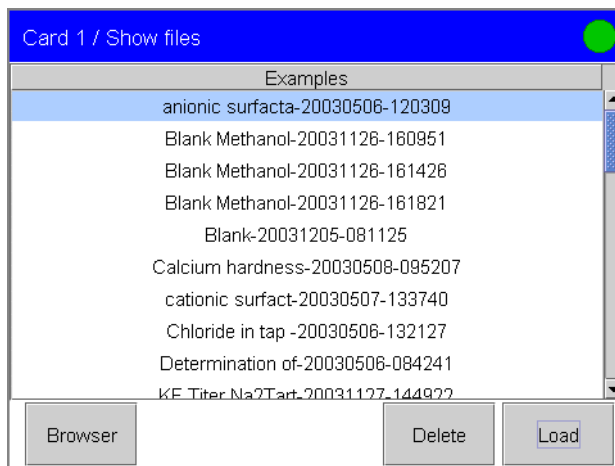
3.18.6 Load determination data

You can load determination files from Card 1, Card 2 or a shared file system (requires 847 USB Lab Link, see *Section 3.10.11*).

- ☞ In the dialog **Results/More determination data** open the selection **Load/Save. Touch Control**: If no card is inserted or no external file system is shared, then the **[Load]** button is inactive.
- ☞ Open the dialog **Load** and select **[Card 1]**, **[Card 2]** or **[Shared memory]** (if present).

☞ Use **[Show all]** to open the list of files containing all the files or **[Show files]** to open the list of files for the selected group. Only determination files will be shown.

In the following example the list of files for the determinations stored under **Examples** is shown. These determinations are stored on Card 1 (**PC Control**) and on the supplied data card with the examples of methods (**Touch Control**).



The selected file is loaded with **[Load]**.



Note!

When you **load a determination** then the method with which the determination was carried out will be loaded automatically. If you have made **alterations to the current method** which you would like to save then you should save the current method before loading the determination.

With **[Delete]** you can remove the selected file from the list of files. If the determination has been automatically saved with write protection, or if **Write protection** has been activated for the determination in the file manager under **Show files/Properties** then it can no longer be deleted.

The **determination browser** allows you to present the determination data more detailed. Not only the determination name is shown in the list but, for example, one of the sample identifications or the method used to carry out the determination and a result. You can also sort the determinations according to various criteria or use a filter. This makes it easier to find the required determination.

☞ Use **[Browser]** to open the browser for the determination files.



Note!

The determination browser always shows only the first **100 files** in the file list. This means that you should take care that not more than 100 files are contained in a single group when arranging the determinations.

Show files / Browser file list

Sorted by Determ. time 17

No.	Identification 1	Result 1
1	water with 5E	0.18 %
2	water in methanol	0.15 %
3	water standard 10	5.2892 mg/mL
4	Calcium hardness	2.300 mmol/L
5	TBN of used motor oil	3.463 mg/g
6	cationic surfactant	0.775 mmol/100g
7	TBN blank value	0.0000 mL
8	Titer SDS	0.9561

Prop-erties Delete Load

Above the list the sorting criterion together with the total number of determinations is shown. Each line corresponds to a determination. The selected file is loaded with **[Load]**. You can remove the selected file from the list of files with **[Delete]**. Under **Browser/Properties** you can select the sorting criterion as well as the data to be shown in the list. You can also use filters on the list.

☞ Open the dialog with **[Properties]**.

Browser / Properties

Contents column1 Identification 1

Contents column2 Result 1

Sort by Determ. time

Sort sequence descending

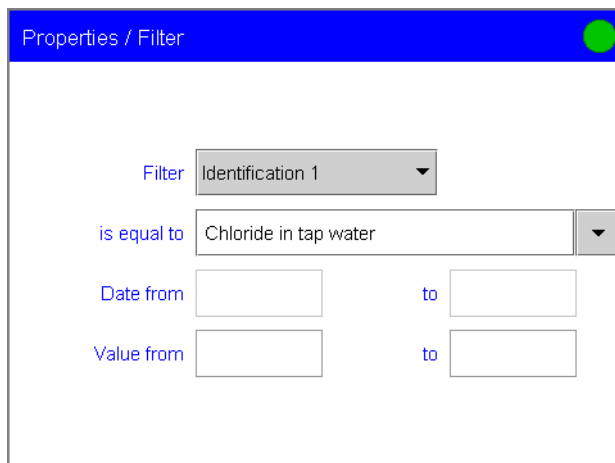
Filter

☞ Select the **Contents** for **Column 1** and **Column 2**. In **Column 1** you can display the sample data (Identification 1 or 2 or the sample size), determination time, method, the result name or the user. In **Column 2** you can choose which result is to be shown. The numbering of the results corresponds to the order in which the results have been calculated in the determination sequence.

☞ Use **Sort by** to select the criterion according to which you want to sort the content of the list. The entries can be sorted by ascending or descending order.

You can set a **Filter** to show the determinations in the browser. A filter is a rule defining what is to be shown.

☞ Open the dialog **Properties/Filter**.

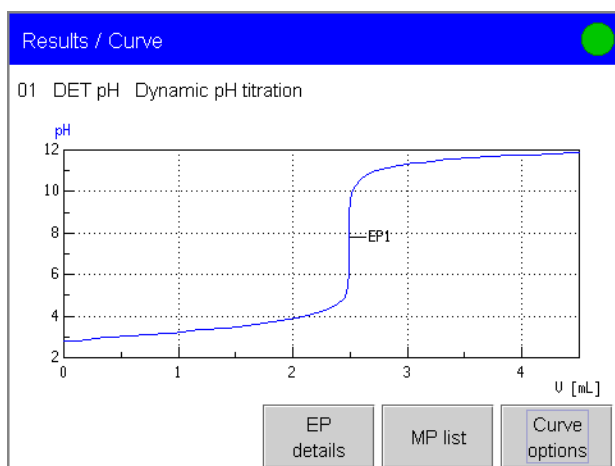


Select a filter criterion under **Filter** and enter the corresponding text or the time range or the range of values in the lines below. The filter can be applied to empty fields as well, for example, if no sample identification has been entered. In this case, select only the desired filter criterion and leave the fields below empty. Only one filter criterion can be active at a time. Only those determinations which meet the filter criterion will be shown in the Browser file list.

3.18.7 Curves

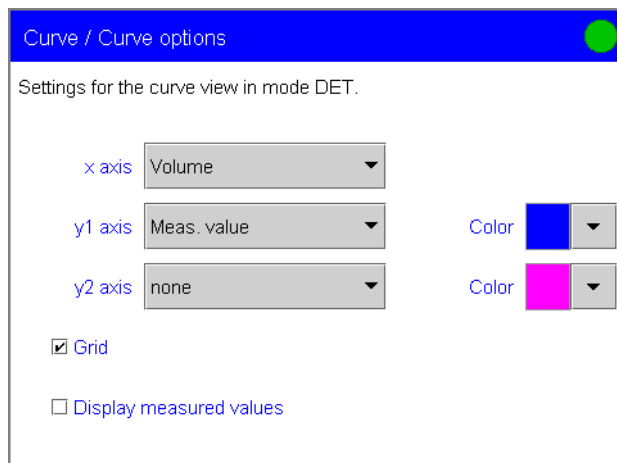
You can open all the curves of the current determination from the **Results** dialog.

- ☞ Use **[Curve]** under **Results** to open the curve view. If the determination contains several modes in which a curve is produced (titration, measurement, calibration, monitored dosing), then a list showing these modes will first be opened. In this case you can select the required curve with **[Show curve]**.



You can alter the presentation of the curve with **[Curve options]**. You can view the **measuring point list** for the curve with **[MP list]**. With **[EP details]** you can view more data for the displayed equivalence points or endpoints. These dialogs are described in *Section 3.18.1*.

- ☞ Open the dialog **Curve/Curve options**.



The settings for the curve view are saved separately and system-specifically for each mode. They apply to the **curve view** under **results** as well as to the **live display** (see Section 3.20.4).

3.18.8 Recalculation and re-evaluation

You can **recalculate** the **results** of a determination

- if you have altered the evaluation parameters in a way that changes the recognized endpoints or equivalence points,
- if you have altered the calculation itself (CALC commands) or
- if variables (e. g. the sample size, titer or common variables) have been altered.



Note!

A **recalculation cannot be undone**. However, you can save the original data by saving the determination before it is recalculated (see Section 3.18.5). The best way of doing this is to use the function **Save automatically** (see Section 3.16.10).

The following commands in the method are executed subsequently with the **[Recalculate]** button in the **Results** dialog:

- For DET and MET titrations the potentiometric evaluation will be carried out again. Under **Edit command/Pot. evaluation** you can alter the parameters for the equivalence point recognition (see Section 4.1.1) and use **[Recalculate]** to start the re-evaluation of the equivalence points (EP). The newly recognized EPs will be shown in the results dialog.
- All subsequent evaluations (**Eval commands**) will be carried out. Under **Parameters/Sequence** (see Section 3.16) you can alter the parameters for the **evaluations** (see Section 4.4) or subsequently insert new evaluations.
- All **calculations (CALC commands)** will be carried out. You can edit the calculations under **Parameters/Sequence** (see Section 3.16) (change formulas, alter result variables, edit result options, etc.; see Section 4.5.1) or insert new calculations. If you subsequently alter the titrant for a titration in a method then the variables TITER and CONC of the "new" titrant will be used in the

calculations. If a result of the variable TITER is assigned in a calculation then the titer of the "new" titrant will also be overwritten.

**Note!**

An alteration of the **calibration data** under **System/Sensors** (see Section 3.9.4) cannot be taken into account in a recalculation. A change of the sensor in a method for a titration or measurement also has no influence on the measured data.

The fact that a determination has been recalculated is shown under **More determination data/Properties** (see Section 3.18.4). The user who was logged in when the recalculation was carried out will also be documented together with the time of the recalculation.

A method may be altered so much, e. g. by the insertion of additional titration commands, that it is no longer possible to recalculate the determination.

Recalculating loaded determinations:

When a loaded determination is recalculated, the titrant data and the common variables stored together with the determination are used. If you want to recalculate the result with a corrected common variable or a corrected titer then you must alter the corresponding values in the dialog **Results/More determination data** under **Local common variables** or **View data/Titrant data**.

**Note!**

With loaded determinations it is assumed that they have been carried out a long time ago and that the **titrant data** and **common variables** of the system no longer coincide with those of the determination. This is the reason why the most important titrant data of the titrants used and the list of common variables (local common variables) are stored together with each determination.

If a result is assigned to the variable TITER or to a common variable then the variables that are currently valid in the system will only be overwritten after a confirmation.

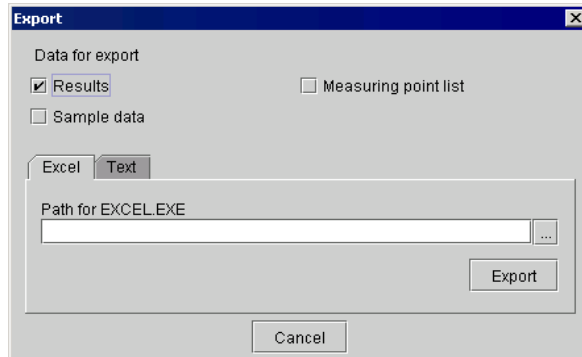
If you subsequently alter the titrant for a titration in the method then this alteration cannot be taken into account in the recalculation.

When loaded determinations are recalculated **no assignments in the result silo** are carried out.

3.18.9 Export (PC Control only)

You can export results, lists of measuring points and sample data of the current determination to Excel or as a text file.

☞ Open the export dialog under **File/Export...**



- **Data for export:** Activate the checkboxes for the data you wish to export.
- **Excel:** Click on Excel if you want to export the data to an Excel table. Press [...] and select the program file EXCEL.EXE in the installation directory of Microsoft Office.
- **Text:** Click on Text if you want to export the data as a TXT file. You must enter the path and the file name including the file extension ".txt". With [...] you can select a folder in which the file is to be stored.

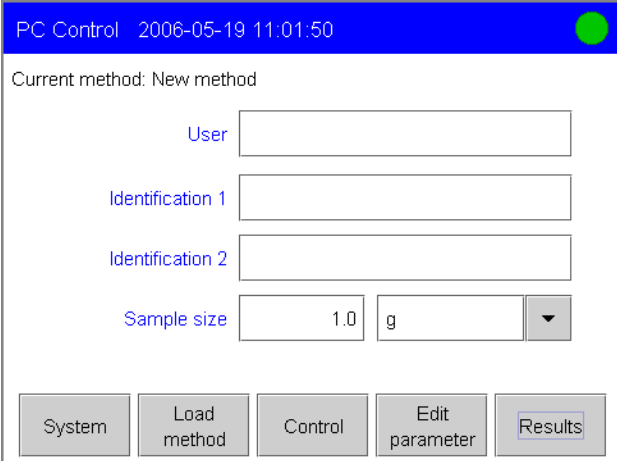
By pressing on [**Export**] the file will be exported in accordance with the settings made above. [**Cancel**] stops the data export.

3.19 Sample data

If you wish to process single samples then you can enter the identifications and sample sizes for the **current sample** directly in the **main dialog**. You can also program an **automatic sample data request** during the determination sequence with a REQUEST command. If you are processing **sample series** then it is a good idea to use the **sample data silo**. The sample data silo is a table in which you can store the identifications, sample size and method with which the sample is to be processed for up to 999 samples.

3.19.1 Sample data input in the main dialog

You can enter the **sample data** for the sample which is to be processed with the next START of a determination (current sample) in the main dialog. You can always access the main dialog with the **[Home]** fixed key. The sample data in the main dialog can also be entered "live", i.e. while a determination is running (see *Section 3.20.5*).



☞ Under **Identification 1** and **Identification 2** you can enter sample-specific data.

The sample identifications can be calculated as the variables **CI1** and **CI2** (see *Section 4.5.7*). The labels of the sample identifications can be edited specifically for the method (see *Section 3.16.6*). Under **System/Templates/Sample data** you can create a **sample identification list**. You can then make a selection from this template when entering the identifications. This simplifies the input of frequently used texts for the identification. You can also enter the identifications with the aid of a barcode reader or send them from a connected balance. With Touch Control we recommend the connection of a PC keyboard if long texts are to be entered as identifications.

☞ Enter the value and unit for the **sample size**.

This value can be calculated as the variable **C00** (see *Section 4.5.7*). The sample size unit can either be selected from a list or entered directly. You can also send the sample size from a connected balance (see *Section 3.10.8*). You can define the **sample size unit** or a **fixed sample size** in the method (see *Section 3.16.6*). The sample size unit

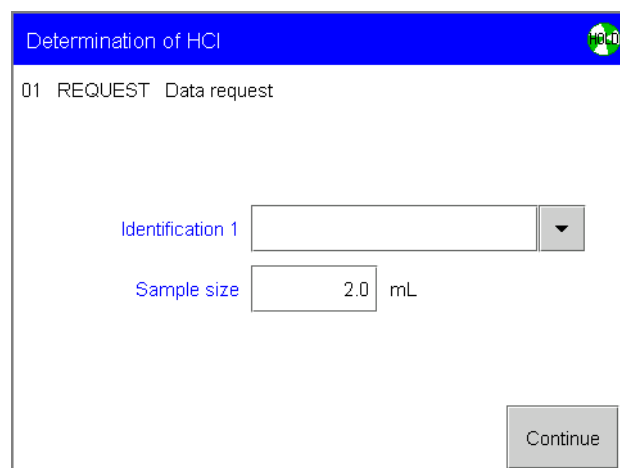
is shown in the main dialog, but can be edited. A fixed sample size cannot be entered in the main dialog. You can also define **sample size limits** in the method which will be monitored during the determination sequence (START of the determination and at the end of the determination) (see Section 3.16.6).

**Note!**

The **sample size limits** are not monitored during the input of the sample data in the main dialog.

3.19.2 Sample data request in the determination sequence

To make sure that the sample data input is not forgotten you can also request the sample data in the determination sequence with a REQUEST command. The automatic sample data request in the determination sequence is essential for back-weighing. In the method you can define which data (Identification 1 and/or 2, sample size) is to be requested (see Section 4.13.3).



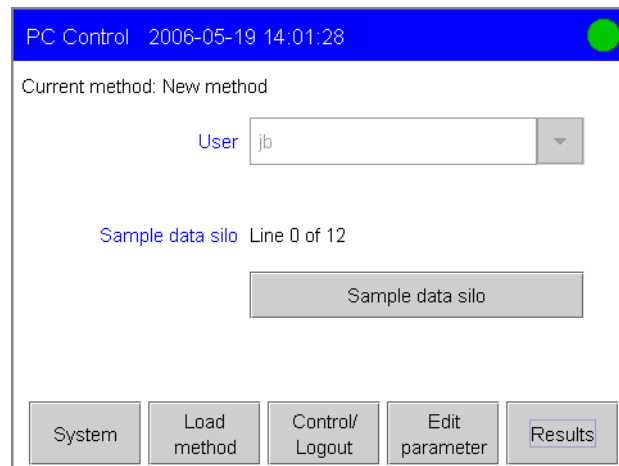
If the **Hold sequence** function is activated in a REQUEST command then the determination sequence will be stopped and must be continued when the sample data has been entered with **[Continue]**. If the **Hold sequence** function is deactivated then the determination will continue in the background until the measured data is required for further processing. The determination will then be held automatically and only continued when the sample data has been entered. In this way you can ensure that the sample data required for calculations carried out after the titration, measurement etc. is actually available. In this case the sample data input is also confirmed with **[Continue]**.

If **sample size limits** have been defined in the method then these will be monitored when the entry has been confirmed with **[Continue]** (see Section 3.16.6). If a **fixed sample size** has been defined in the method then the sample size will be shown during the input of the sample data but cannot be edited (see Section 3.16.6).

3.19.3 Sample data silo

If you would like to use the sample data silo then you must activate the corresponding checkbox under **Control**. With **PC Control** you can also enter the sample data when the sample data silo has not been activated. You can open and close the table in the menu **View**. With **Touch Control** the sample data silo for the sample data input must be activated.

If the sample data silo is activated then in the main dialog the **[Sample data silo]** button will be seen instead of the input field for the sample data.

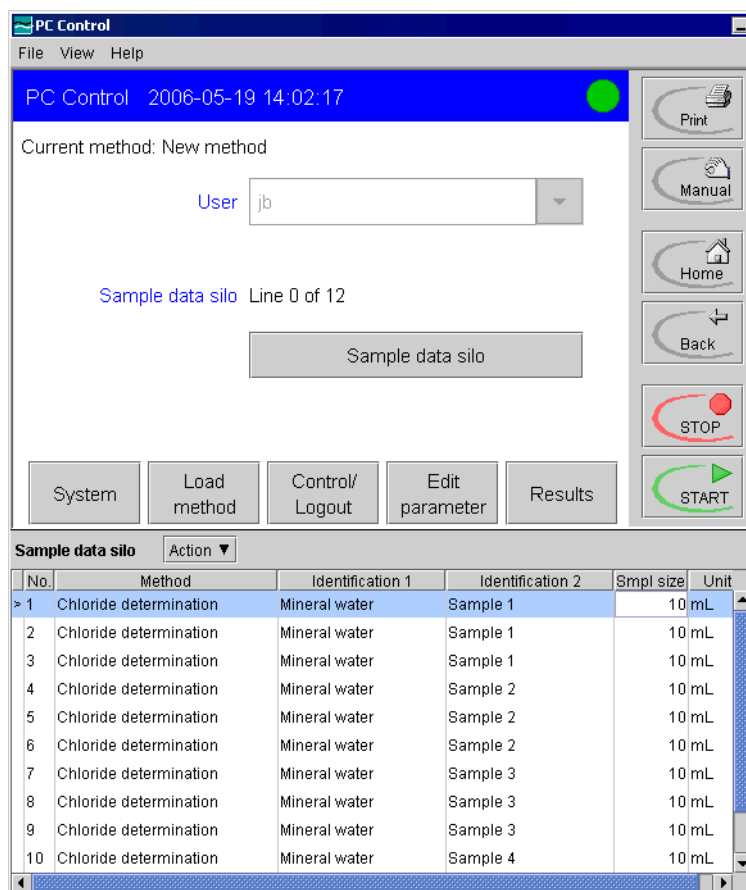


For the **sample data silo** the number of lines which have already been processed from the total number of lines in which sample data have been entered is shown in the main dialog.

☞ Open the sample data table with **[Sample data silo]**.

PC Control

With PC Control the sample data table is shown beneath the open dialog window. The individual fields can be filled in directly. The silo line into which the weight is transmitted by a balance is indicated by the following character: >.



Click on **Action** in the title line of the sample data silo.

Insert line
Delete line
Delete all silo lines
Load sample data silo
Save sample data silo
Reset line number
Silo line for balance
Properties
Show Help
Close

You can use **Insert line** to insert a new silo line in front of the selected line, delete the selected line with **Delete line** and clear the whole of the current silo with **Delete all silo lines**. The settings under **Sample data silo/Properties** are retained.

You can use **Load sample data silo** to open the dialog for loading a sample data silo file and **Save sample data silo** to open the dialog to save the current sample data silo. The procedure how to load and save is described on *page 151*.

When all the existing silo lines have been processed and you would like to refill the sample data silo then you can use **Reset line number** to set the first line back to No. 1. With **Silo line for balance** you can mark the selected silo line (>), into which the weight transmitted by a balance is to be entered. If the sample data input for the silo line is concluded automatically (see *p. 150*) then the marking will be automatically set in the next line.

With **Properties** you can open the dialog **Sample data silo/Properties** (see *p. 149*); **Show help** opens the online help for the sample data silo and **Close** is used to close the sample data table again.

Touch Control

With Touch Control a new dialog window is opened to show the sample data silo. Apart from the column with the line number, a maximum of

two further columns can be shown. The columns to be shown is defined under **Sample data silo/Properties** (see p. 149).

Sample data silo			
No.	Identification 1	Sample size	
1	Mineral water	10 mL	▲
2	Mineral water	10 mL	
3	Mineral water	10 mL	
4	Mineral water	10 mL	
5	Mineral water	10 mL	
6	Mineral water	10 mL	▼



Note!

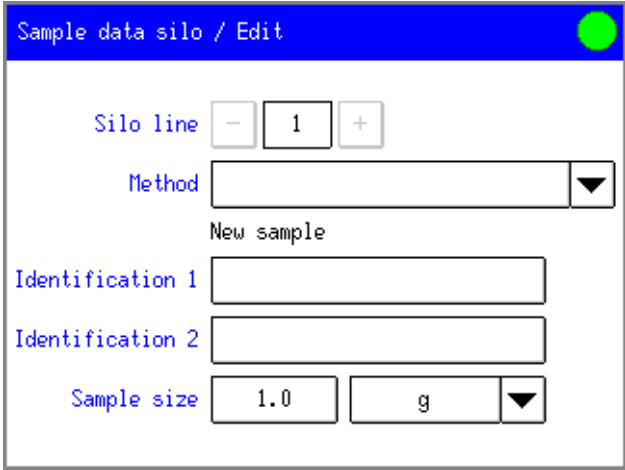
Sample data silo files can be exchanged between **PC Control** and **Touch Control** as their contents are identical.

With **[Edit]** you can open the dialog in which the data for the selected line is to be entered. **[Delete]** is used to delete the selected silo line. With **[Insert Line]** you can insert an empty silo line in front of the selected silo line.

The sample data is entered and processed line by line in ascending order. The **"active" line** which is currently being processed (current sample) has a yellow background with PC Control; with Touch Control it is indicated by the text being shown in green.

The input of the individual sample data (Identification 1, Identification 2, value and unit for the sample size) and the method is in principle the same for PC Control and Touch Control. In PC Control the data is entered directly into the table, in Touch Control a new dialog is opened for editing the silo line.

☞ With **Touch Control** open the edit dialog for the selected silo line with **[Edit]**. If you want to fill an empty sample data silo then this is the first empty silo line. In the first line you can see which line you are currently editing. The new line will only be saved when the entry is confirmed. As long as the line has not been saved **New sample** will be shown under the input field for the method name. In the edit dialog for the active line which is currently being processed **Current sample** will be shown in the same place. If several silo lines are already present you can use the **[+]** and **[-]** buttons to switch between the edit dialogs for the individual lines without having to return to the table.



You should now enter the sample data, irrespective of whether you are using PC Control or Touch Control.

- ☞ Under **Method** you can select the name of the method with which the sample is to be processed. You can use **Sample data silo/Properties** to define the **Method memory** (internal memory, Card 1, Card 2, Shared memory) from which the method is to be loaded. You can also enter the method name. If no method is entered then the current method will be used. If you enter the same method in successive silo lines then the method will not be loaded separately for each determination.

If you have switched on the use of the **Sample assignment table** under **System/Templates/Sample data** then you cannot define a method in the sample data silo. If a method has already been entered before the sample assignment table is activated then this entry will be ignored.

- ☞ You can enter sample-specific data under **Identification 1** and **Identification 2**.

The sample identifications can be accounted as the variables **CI1** and **CI2** (see *Section 4.5.7*). The labels of the sample identifications can be edited specifically for the method (see *p. 150*). Under **System/Templates/Sample data** you can create a **sample identification list**. You can then make a selection from this template when entering the identifications. This simplifies the input of frequently used texts for the identification. You can also enter the identifications with the aid of a barcode reader or send them from a connected balance. With Touch Control we recommend the connection of a PC keyboard if long texts are to be entered as identifications.

- ☞ Enter the value and unit for the **sample size**. If you have retained the standard settings under **Sample data silo/Properties** then the silo line will be concluded with the sample size. With PC Control if you confirm the input of the value with **[Enter]** then a new silo line will be generated automatically. With Touch Control if you confirm the input of the value with **[OK]** then the program will automatically change to the edit dialog for the next silo line.

The value for the sample size can be calculated as the variable **C00** (see *Section 4.5.7*). The sample size unit can either be selected from a

list or entered directly. You can also send the sample size from a connected balance (see Section 3.10.8). If you have defined a **sample size unit** (see Section 3.16.6) then this will be ignored in the sample data silo. The sample size unit entered in the sample data silo will always be used. If you have defined a **fixed sample size** (see Section 3.16.6) then this will be written into the corresponding silo line when the method is opened. The previously entered sample size (this is usually still the default value of 1.00 g) will be overwritten.

You can also define **sample size limits** in the method; these will be monitored in the determination sequence (see Section 3.16.6).

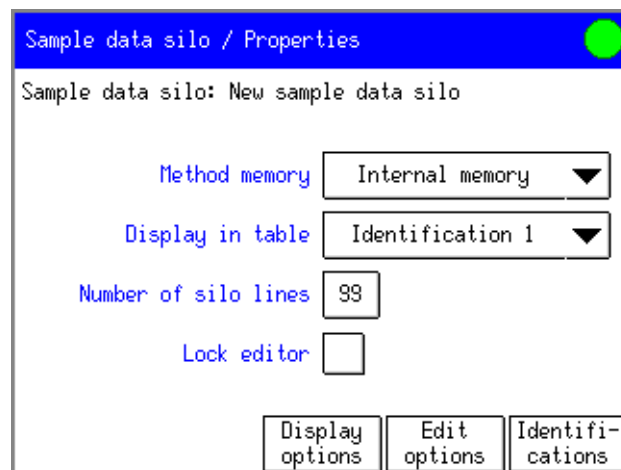


Note!

The **sample size limits** are not monitored during the input of the sample data in the sample data silo.

Properties of the sample data silo

☞ Open the dialog **Sample data silo/Properties**. With PC Control this is done by selecting the menu item **Properties** under **Action** (see p 146). With Touch Control open the corresponding dialog from the sample data silo table with **[Properties]**.



The details of the dialogs **[Display options]**, **[Edit options]** and **[Identifications]** are described on the following pages.



Attention!

With **PC Control** the settings made under **Sample data silo/Properties** and its subdialogs will only become effective when the dialog is changed, e. g. with **[Back]**.

- ☞ Under **Method memory** select the memory location from which the methods for carrying out the determinations are to be loaded.
- ☞ **Touch Control**: choose whether **Identification 1 or 2** and the **sample size** or only the **method** is to be shown in the silo table. With PC Control all the columns are always shown.
- ☞ You can enter the maximum **Number of silo lines**. When this number of lines has been entered the silo is full and no further lines can be added.

- ☞ You can **disable editing** the sample data in the sample data silo. This is a good idea when the sample data silo has been filled and you wish to prevent data from being altered while the silo is being processed.

Display options (Touch Control only)

- ☞ Open the dialog **Properties/Show options** and deactivate the checkboxes for the sample data you do not want to use. These will then no longer be shown in the edit dialog for the individual samples.

Edit options

In this dialog you can define the settings for editing the sample data table.

- ☞ Open the dialog **Properties/Edit options**.



- ☞ Select whether the silo line is to be automatically concluded with **Sample size**, **Identification 1** or **Identification 2**. When the corresponding entry is confirmed with **[OK]** or **[Enter]** then the program switches automatically to editing the next line. You can also conclude the sample data input for a silo line **manually**. With **Touch Control** in this case the **[New sample]** button will be shown in the edit dialog. With that you can open the edit dialog for a new sample. With **PC Control** a new silo line will be generated when the sample size is confirmed with **[Enter]**.
- ☞ If you have to enter similar data for each sample then you can **automatically copy into the next line** the data which is identical for each sample. Deactivate the checkboxes for the data which is not to be copied into the next line.

Identifications

If you want to enter different method-independent labels for the identifications, e. g. batch number, density, etc. then you can enter your own labels under **Label1**. These will be updated in the sample data table and when the sample data is requested with a REQUEST command.

- ☞ Open the dialog **Properties/Identifications**.

Save sample data silo

Sample data silo files can only be saved on Card 1, Card 2 or a shared file system (requires 847 USB Lab Link, see *Section 3.10.11*).

- ☞ Open the selection **Load/Save** in the dialog **Sample data silo**.
Touch Control: If no card is inserted or no external file system is shared, then the **[Save]** button is inactive.
- ☞ Open the dialog **Save**. The procedure for saving a file is described in *Section 3.11.4*

Load sample data silo

Sample data silo files can only be loaded from Card 1, Card 2 or a shared file system (requires 847 USB Lab Link, see *Section 3.10.11*).

- ☞ Open the selection **Load/Save** in the dialog **Sample data silo**.
Touch Control: If no card is inserted or no external file system is shared, then the **[Load]** button is inactive.
- ☞ Open the dialog **Load** and select **[Card 1]**, **[Card 2]** or **[Shared memory]** (if present).
- ☞ Use **[Show all]** to open the list of files containing all the files or **[Show files]** open the list of files for the selected group. Only sample data silo files will be shown.

You can load the selected file with **[Load]**. The program then switches automatically to the main dialog. You can remove the selected file from the list of files with **[Delete]**.

3.19.4 Export of sample data

The export of the sample data of the current determination is described in *Section 3.18.9*.

3.20 Determination sequence

This section provides a description of how to **carry out a determination**, i.e. how to process a **single sample** or a **sample series**. The determination sequence is defined in the method. When a determination is started the current method is processed line by line. The current sample data is used for calculations.

3.20.1 Carrying out a single determination

If you wish to process a single sample then proceed as follows:

- ☞ Load the **method** with which the sample is to be processed (see *Section 3.15.1*).
- ☞ Enter the **sample data** in the main dialog (see *Section 3.19.1*).
- ☞ Start the determination sequence with the **[START]** fixed key.



When a determination has been started a check is first made that all **devices** which are necessary are connected and ready for use and whether all the titrants are present. All the **monitoring intervals** for the titrants, sensors and common variables are also checked. Then all the **method commands** are processed in succession. The dialog changes automatically to the **live display** (see *Section 3.20.4*). While a determination is being carried out this is indicated by a **moving symbol** in the status line. When all the method commands have been processed the determination is concluded and the program switches automatically to the **Results** dialog (see *Section 3.18*). Only if you alter the live parameters, edit the sample data silo (Touch Control only) or if the manual control window is open (Touch Control only) will there be no automatic switch to the results display at the end of the determination. You can see when the determination is finished from the status display at the top right corner.



In case results of the determination are saved in the **result silo** they will be copied into the result silo at the end of the determination (see *Section 3.22*).

If you have switched on the use of the **sample assignment table** (see *Section 3.14.2*) then a check will be made at START whether the identification which has been selected as the assignment identification is present in the sample assignment table. If this is so then the assigned method will be loaded automatically and the determination itself will be started. If the automatic request for the assignment identification is switched on this will be requested first.

3.20.2 Processing a sample series

You can use the following functions when processing sample series:

Statistics for multiple determinations:

☞ Activate the **Statistics** checkbox in the method under **Options Method** and enter the **Number of samples** whose results are to be used for the statistical calculations. You can carry out the determinations individually or use the sample data silo for entering the sample data (see below).



Note!

Only results that have been produced with the same method can be used in the statistics.

Sample data silo: in the sample data silo you can enter the sample data for a whole sample series and process the series in succession.

☞ Activate the use of the **sample data silo** under **Control** (see Section 3.17.2).

☞ Enter the **sample data** in the sample data silo. You can also edit the sample data silo "live", i.e. while a determination is being carried out. You can define the **method** used to process each sample in the sample data silo. This is not necessary if all samples are to be processed by the same method. In this case the current method will be used.



There are various ways of starting the determination of a sample series.

- You can start the sequence for each individual determination with the **[START]** fixed key.
- You can use the **autostart** function, which can be activated under **Control** (see Section 3.17.3). In this case the next determination will be started automatically after the end of the previous one.

If a **method** is entered in the sample data silo then this method will first be loaded and then the determination sequence will be started.

When a determination has been started a check is first made that all **devices** which are necessary are connected and ready for use and whether all the titrants are present. All the **monitoring intervals** for the titrants, sensors and common variables are also checked. Then all the **method commands** are processed in succession. The dialog changes automatically to the **live display** (see Section 3.20.4). While a determination is being carried out this is indicated by a **moving symbol** in the status line. When all the method commands have been processed the determination is concluded and the program switches automatically to the **Results** dialog (see Section 3.18). Only if you alter the live parameters, edit the sample data silo (Touch Control only) or if the manual control window is open (Touch Control only) will there be no automatic switch to the results display at the end of the determination. You can see when the determination is finished from the status display at the top right corner. The sample data from the processed sample



data silo line is copied into the determination file and the line in the sample data silo is deleted.

In case results of the determination are saved in the **result silo** they will be copied into the result silo at the end of the determination (see *Section 3.22*).

If you have switched on the use of the **sample assignment table** (see *Section 3.14.2*) then a check will be made at START whether the identification which has been selected as the assignment identification is present in the sample assignment table. If this is so then the assigned method will be loaded automatically and the determination itself will be started. If methods have been entered for the sample data in the sample data silo then these entries will be ignored.

3.20.3 Stopping determinations manually



A determination can be stopped at any time with the **[STOP]** fixed key. The command which is being processed will be stopped and no further commands will be carried out. The program will switch automatically to showing the **Results** (see *Section 3.18*).

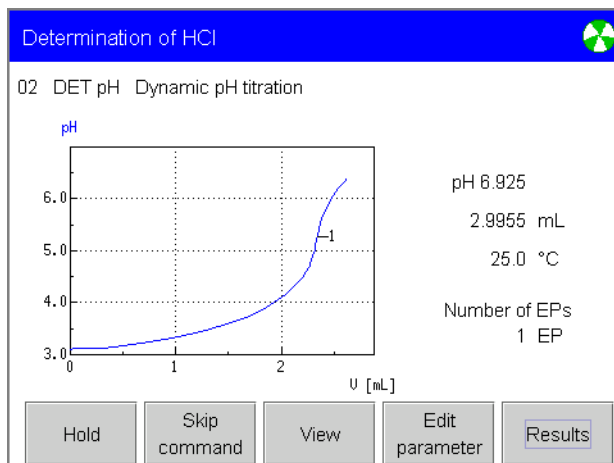
If the **autostart** function is switched on (see *Section 3.17.3*) then the processing of the whole series will be stopped and no further automatic START will be carried out.

If you do not want to stop the whole determination sequence but only want to stop a command then you should use the function **[Skip command]** in the live display (see *Section 3.20.4*). This is particularly useful when you want to stop a titration because the required equivalence point has already been found. All the following commands, e. g. calculations and report printouts, will still be carried out.

3.20.4 Live display

In each method command which is processed in the determination sequence and which lasts for a certain time the step which is currently being carried out is indicated. The name of the current **method** is shown in the **status line** (blue bar). In the first line the line number, **command name** and **command comment** are shown for the command which is currently being processed.

The corresponding curve is shown for titrations, measurements and for the monitored dosing. If you have selected the presentation of **Curve & measured values** under **View** then to the right of the curve you will see the number of equivalence points or endpoints (EP) which have been recognized in addition to the measured values. The endpoints are marked on the curve.



With **[Results]** you can open the results display. The data for the method commands which have already been carried out will be shown. The **Results** dialog and its subdialogs will not be updated during the sequence as long as they are open. If you want to view the most recent results you must exit the dialog and then reopen it.

With **[Edit parameter]** you can edit the live parameters, i.e. the method parameters which can be altered while a sequence is being processed (see Section 3.20.6).

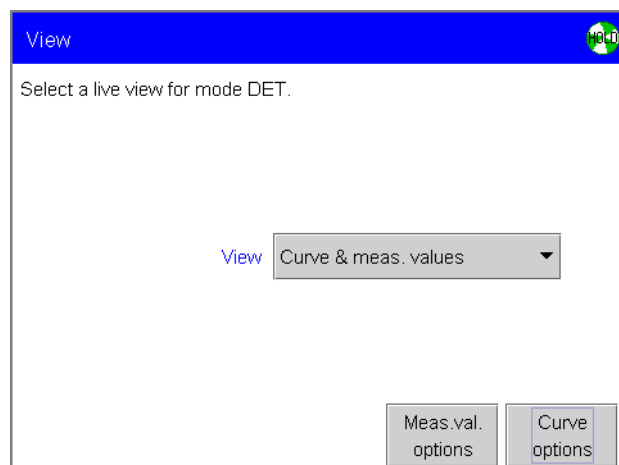
The button in the center has various functions. For titrations and measurements as well as for the monitored dosing you can use **[View]** to make settings for displaying the curve and the measured values (see below). In the live display for all commands you can switch to the main dialog with **[Sample data]**.

With **[Skip command]** the method command which is currently being processed will be stopped. The sequence will be continued with the next command. If a titration, measurement, calibration or monitored dosing is stopped with **[Skip command]** then the determination data will show **Manual stop** as the stop criterion.



With **[Hold]** you can halt the determination at any time. The system is then in the HOLD status (status display in the top right corner). The button marking then changes to **[Continue]**. You can use **[Continue]** to continue the sequence.

☞ Use **[View]** in the live display to open the dialog for a titration, measurement or monitored dosing in order to alter the settings for showing the curve and measured values.



You can choose whether you would like to display the curve with the measured values to the right of it (default setting), only the curve (larger, fills the whole display), only the measured values (large) or the curve with the sample data to the right of it.

You can alter the appearance of the curve with **[Curve options]** (see *Section 3.18.7*). The settings for the curve display are stored separately and system-specifically for each mode. They apply both to the **curve display** under **results** and the **live display**.

With **[Measured value options]** you can alter the display of the measured values. A maximum of three different values can be shown at the same time. The values which can be selected vary with the mode.

The CAL (**calibration**) command has a special sequence and is described in *Section 4.7*.

For the ADD (**dosing**) command the volume to be added (set volume) and the volume already added are shown. For the PREP (**preparation**) and EMPTY (Dosino only) commands the piston movements and the valve settings are shown.

For the **SCAN** command the signal which is being waited for is shown.

For the WAIT (**waiting time**) command the remaining waiting time is shown, possibly together with a message which can be defined in the method.

For all other command a text is either shown or they are carried out so quickly that no special live display is available (e.g. evaluations, calculations, etc.).

3.20.5 Main dialog "live"

The appearance of the main dialog changes slightly when a determination has been started.

The **sample data** can also be entered "live", i.e. while a determination is being carried out (see *Section 3.19.1*). In calculations the sample data which has been entered in the main dialog at the time when the calculation is carried out (CALC command) is always used.

No device-specific settings can be carried out "live"; this is why the **[System]** button is not available. It is also not possible to load or create methods. The **[Load method]** button is also not available.



With **[Hold]** you can halt the determination at any time. The system is then in the HOLD status (status display in the top right corner). The button marking then changes to **[Continue]**. You can then use **[Continue]** to continue the sequence.

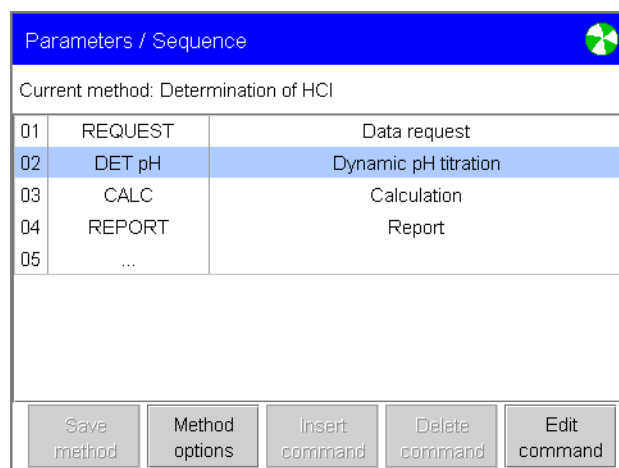
You can switch to the live display with **[Live display]**, i.e. to showing the method command which is currently being processed.

With **[Control]** you can alter the settings for the determination sequence (see *Section 3.17*). Several functions are not accessible "live". The settings for **Statistics** and **Sample data silo** cannot be altered. If you deactivate the **Autostart** checkbox while a determination is being carried out then the current determination will be concluded but no new START will be carried out. The sample number cannot be edited. If you are working with login (see *Section 3.7.7*) then you can log out of the system with **[Logout]** even when a determination is being carried out. The logout dialog will then be shown immediately. The determination continues to run in the background. It can be stopped with the **[STOP]** fixed key. All other functions are only accessible again after a new user has logged in.

3.20.6 Live parameters

Certain method parameters can be edited while a determination is being carried out.

- ☞ Open the **Edit parameter** dialog while a determination is currently being carried out.

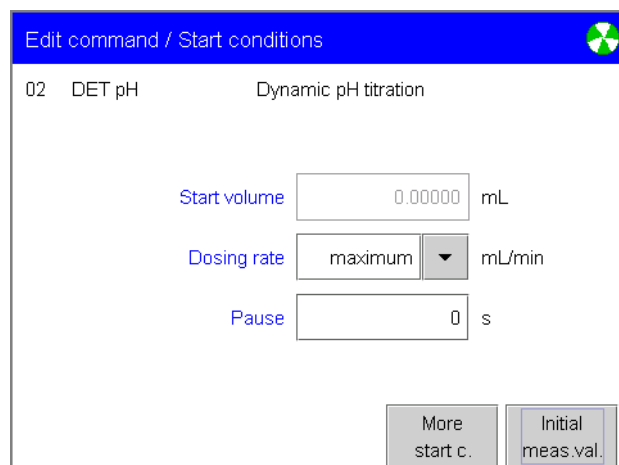


Parameters / Sequence		
Current method: Determination of HCl		
01	REQUEST	Data request
02	DET pH	Dynamic pH titration
03	CALC	Calculation
04	REPORT	Report
05	...	

Save method Method options Insert command Delete command Edit command

The **[Edit command]** button is active for a command in which live parameters can be edited. The sequence, i.e. the sequence of commands, cannot be altered. This is why the **[Delete command]** and **[Insert command]** buttons are inactive. Under **Method options** all functions are accessible except the method properties. The method cannot be saved while a determination is being carried out.

- ☞ As an example, open the dialog for editing the **Start conditions** for a DET titration.



Edit command / Start conditions

02 DET pH Dynamic pH titration

Start volume mL

Dosing rate mL/min

Pause s

More start c. Initial meas.val.

Only parameters which it is possible to edit while a determination is being carried out can be edited.

The edited parameters are immediately taken into account in the determination sequence. However, for example, if you alter the start conditions after the start volume has already been added then these alterations will only be taken into account the next time that the method is started.

**Note!**

*If the **sample data silo** is used and a different method is loaded for the next sample then the live alterations will be lost.*

3.21 Statistics

In the **Results** dialog you can open the statistics overview of a multiple determination with **[Statistics]**. A maximum of nine results calculated in a single determination can be statistically evaluated. A statistics series can contain a maximum of 20 determinations, i.e. samples.

If you wish to have statistical calculations carried out on the results then you have to activate the **Statistics** checkbox in the method under **Sequence/Method options** and enter the **Number of samples** (see Section 3.16.4).

The results for which statistical calculations are to be carried out are defined in the **CALC command** (calculation).

You find a short description about statistical calculations in the **Tutorial** for Touch Control and PC Control.

Results / Statistics	
Current method: New method	
Determinations 3 of 3	
Result name	Mean
Content (mmol/L)	99.86 mmol/L
Volume HCl	5.1 mL
<div style="display: flex; justify-content: space-between; margin-top: 10px;"> Add determ. Details </div>	

The number of determinations that have already been carried out is shown above the list (actual statistics counter) together with the total number of determinations to be carried out (set statistics counter). The name of the result and the mean value are shown for each result.

With **[Details]** you can display the statistics results for the selected result and the individual results of all the determinations. With **[Add determination]** you can also add a sample to the series later. This is a good idea if one determination in the series was so incorrect that it cannot be accepted.



Note!

If you **recalculate** a **determination** then the statistics calculations for the determination will also be recalculated.

3.21.1 Statistical information about the result

Select a result and press **[Details]**.

Statistics / Details		
Result name: Content (mmol/L)		SMN1
Mean	99.86 mmol/L	n=03
s +/-	0.087 mmol/L	
s rel	0.09 %	
No.	Sample size	Result
1	5.1 mL	99.93 mmol/L
2	5.5 mL	99.76 mmol/L
3	4.8 mL	99.88 mmol/L
<input type="button" value="Sample data"/> <input type="button" value="Determ. on/off"/> <input type="button" value="Result on/off"/>		

The name of the result and the variable for the mean value (in this example **SMN1**) are shown under **Details** for each result (see Section 4.5.1). The **Mean** value and the absolute (**s +/-**) and relative (**s rel**) standard deviation are also shown above the list. The number of individual results used for the calculation of the mean value is shown to the right of the mean value. The number of the determination, the sample size and the value including unit are shown in the list for each result.

Results that could not be calculated are indicated with **invalid** and will be ignored.

You can use **[Result on/off]** to exclude individual results from the statistical calculations. The value for this result will then be indicated by an *****. With **[Determination on/off]** you can exclude all the results of a determination from the statistical calculations. In this case, all the entries in the corresponding line will be indicated by an *****. The statistical results will be recalculated immediately. You can use the same buttons to undo these actions again. If you have assigned the mean value to a **common variable** or to the variable **TITER** (see Section 4.5.1) then you have to recalculate the determination (see Section 3.18.8).

Identification 1, **Identification 2** and the **Sample size** of the selected determination are shown under **Details/Sample data**.

3.21.2 Delete statistics data

You can delete the whole statistics data manually under **Control** with **[Delete statistics]**.

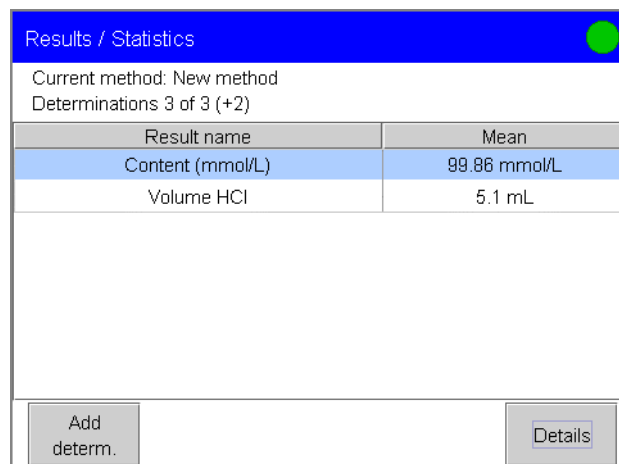
The statistics data is deleted automatically in following cases:

- when the actual statistics counter (number of processed samples) is the same as the preset number of determinations used for the statistics. The maximum value of the statistics counter is defined under **Sequence/Method options**.
- when a method is loaded with **[Load method]**. It does not matter whether this is the same method that was previously loaded. If you use either the sample data silo or the sample assignment table then a check will be made whether the method is the same (file name is the same) as that already loaded. Only when this is a different method will the new method be loaded and the statistics deleted.

3.21.3 Adding a determination to a statistics series

You can add an additional sample to a statistics series because, for example, another sample had to be excluded from the statistics. In this case, increase the set statistics counter under **Results/Statistics** with **[Add determination]**. This does not alter the **Number of samples** defined in the method under **Sequence/Method options**. When the required number of determinations has been carried out the set statistics counter defined in the method will again apply to the next statistics series.

The number of determinations by which the set statistics counter has been increased is shown above the list in brackets. This modification is also shown in the main dialog and in the statistics report.



Result name	Mean
Content (mmol/L)	99.86 mmol/L
Volume HCl	5.1 mL

3.22 Result silo

The result silo is ideal for providing a clear overview of the results carried out, for example, on a particular day. You can store the **results of up to 200 determinations**. A maximum of nine results from a single determination can be stored in the result silo. As the display is not large enough to show all the data at the same time, it is a good idea to print out the result silo (see *Section 3.23*).

The results that are to be stored in the result silo are defined in the **CALC command** (calculation).

In the **Results** dialog you can open the result silo with **[Result silo]**.

No.	Identification 1	Result 1
1	Titer NaOH	0.9967
2	Titer NaOH	0.9944
3	Titer NaOH	0.9976
4	Batch 1	0.124 mol/L
5	Batch 1	0.125 mol/L
6	Batch 1	0.128 mol/L

The criterion according to which the results have been sorted is shown above the list together with the number of determinations (of max. 200) from which results have been stored in the result silo. If a filter has been used then this number will normally be higher than the number of lines shown. Each line corresponds to a determination.

The following details of the determination can be viewed with **[Details]**:

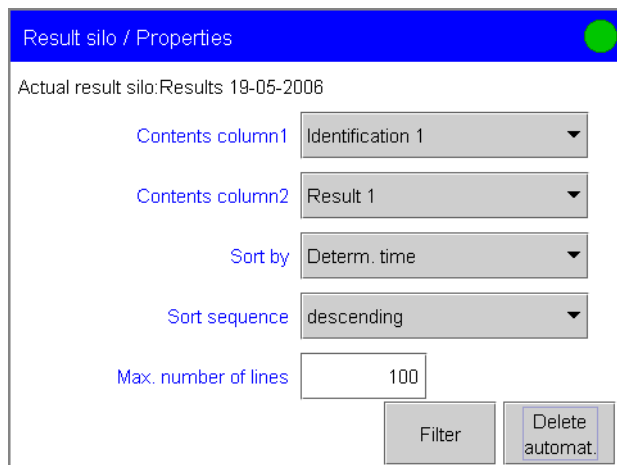
- User who carried out the determination.
- Method with which the determinations was carried out.
- Determination time (date and time).
- Sample data (Identification 1 and 2, sample size).
- Results which have been calculated in the determination sequence and stored in the result silo.

The selected determination line can be deleted from the result silo with **[Delete]**. **[Delete all]** deletes all the lines.

3.22.1 Properties of the result silo

Under **Result silo/Properties** you can choose the criteria according to which the list is to be sorted and the data to be shown for each determination.

☞ Open the dialog with **[Properties]**.



☞ Select the **Contents** of **Column 1** and **Column 2**. In **Column 1** you can display the sample data (Identification 1 or 2, or sample size), determination time, method, the name of the result or the user. In **Column 2** you can select the result to be shown. The numbering of the results corresponds to the order in which the results have been calculated in the determination sequence and stored in the result silo. The numbering does not correspond to the result variable to which the result has been assigned.

☞ Use **Sort by** to select the criterion according to which you want to sort the content of the list. The entries can be sorted in ascending or descending order.

☞ The maximum number of lines in the result silo can be defined under **Max. number of lines**. If a result silo containing more lines than defined here is imported (loading or backup), the maximum number of lines is increased to that value.

With **[Delete automatically]**, you define when the contents of the result silo is deleted automatically. You can set it so that the oldest silo line will be deleted when the result silo is full and a new determination is to be entered. All lines can be deleted automatically when the titration system is switched on, when a new sample series is started with the autostart function switched on or when the result silo is saved.

You can use **filters** for the display of the result silo table. A filter is a rule defining what is to be shown.

☞ Open the dialog for selecting the filter criteria under **Result silo/Properties** with **[Filter]**.

Properties / Filter

Filter Identification 1


is equal to Titer NaOH

Date from [] to []

Value from [] to []

Select a filter criterion under **Filter** and enter the corresponding text or the time range or the range of values in the lines below. The filter can be applied to empty fields as well, for example, if no sample identification has been entered. In this case, select only the desired filter criterion and leave the fields below empty. Only one filter criterion can be active at a time. Only those determinations which meet the filter criterion will be shown in the result silo:

Results / Result silo

Sorted by Determ. time 6 of 200 

No.	Identification 1	Result 1
1	Titer NaOH	0.9987
2	Titer NaOH	0.9944
3	Titer NaOH	0.9976

Load/ Save Properties Delete all Delete Details

The fact that a filter is active is indicated by the filter symbol in the top right-hand corner.

3.22.2 Saving and loading the result silo

Save result silo

Result silo files can only be saved on Card 1, Card 2 or a shared file system (requires 847 USB Lab Link, see *Section 3.10.11*).

- ☞ Open **[Load/Save]** in the dialog **Results/Result silo**. Touch Control: If no card is inserted or no external file system is shared, then the **[Save]** button will be inactive.
- ☞ Open the **Save** dialog. The procedure for saving a file is described in *Section 3.11.4*.



Note!

*Not all determination data are saved with a result silo. If you want to save determination data of all determinations, use the option **Save determination automatically** (see *Section 3.16.10*).*

Load result silo

Result silo files can only be loaded from Card 1, Card 2 or a shared file system (requires 847 USB Lab Link, see *Section 3.10.11*).

- ☞ Open **[Load/Save]** in **Results/Result silo**. Touch Control: If no card is inserted or no external file system is shared, then the **[Load]** button will be inactive.
- ☞ Open the dialog **Load** and select **[Card 1]**, **[Card 2]** or **[Shared memory]** (if present).
- ☞ Use **[Show all]** to open the list of all the files or **[Show files]** to open the list of files for the selected group. Only result silo files will be shown.

You can use **[Load]** to load the selected file. You can remove the selected file from the list of files with **[Delete]**.

3.23 Print

In principle there are two ways of printing a report in Touch Control and PC Control:

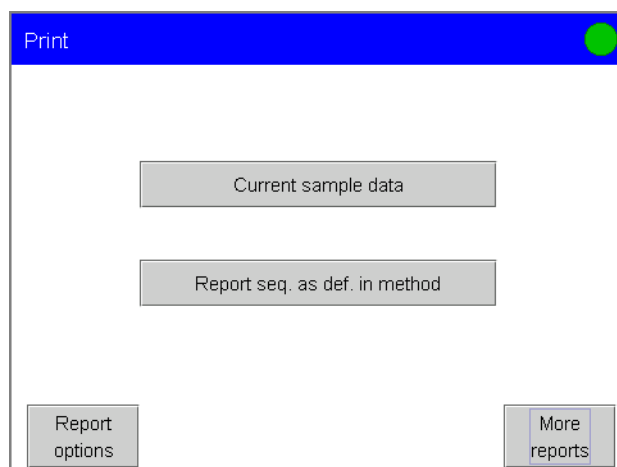
- Manual printout with the **[Print]** fixed key (see below).
- Printout during the determination sequence with a **REPORT command** (see *Section 4.6*).

By using the **PC Control** software you have the additional possibility to generate reports directly as PDF file. The settings are described on *page 175*.

How to connect a printer to a Titrando system with **Touch Control** is described in the Installation Instructions for the Titrando. The configuration of the printer is described in *Section 3.10.7*. The **PC Control** software automatically uses the printer selected under File/Printer.

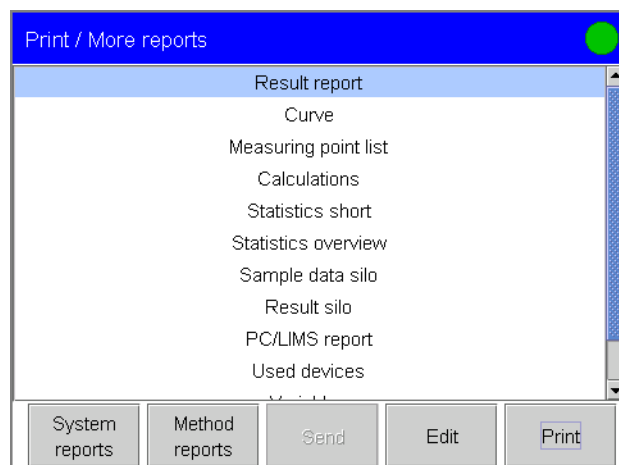
You can use the **[Print]** fixed key to rapidly print out **context-sensitive** reports for the dialog which is currently open. You can also print out all other reports which are available. The **[Print]** fixed key is inactive while a determination is being carried out (BUSY).

☞ Open the **Print** dialog from the main dialog with the **[Print]** fixed key.



The sample data is entered in the main dialog, which is why you can print out the sample data from the main dialog in a context-sensitive situation with **[Current sample data]**. All reports as defined in the current method can be printed with **[Report seq. as def. in method]**. With **[More reports]** you can open a list containing all the available reports. You can make general settings for printing out the reports with **[Report options]**.

☞ Open the dialog **Print/More reports**. The first list shows the reports for the current determination.

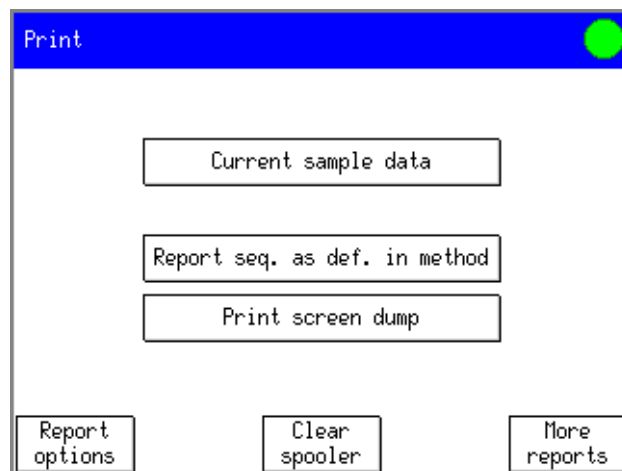


The selected report can be printed out with **[Print]**. With **[Edit]** the parameters for the printout can be edited for some reports. The **[Send]** button is only active when **PC/LIMS report** has been selected. **[Method reports]** opens the list of reports for the current method. The list containing all the reports about the system-specific data is opened with **[System reports]**.

If the **[Print]** fixed key is used then the reports will always be printed out with the **default settings**. If you wish to print out a report with different settings then you should define a REPORT command in the method and adapt the parameters for the report (see *Section 4.6*). The report defined in the method is printed out with **[Print] [Report sequence as defined in method]**.

With **Touch Control** you can also print out a **screen dump** of the current dialog.

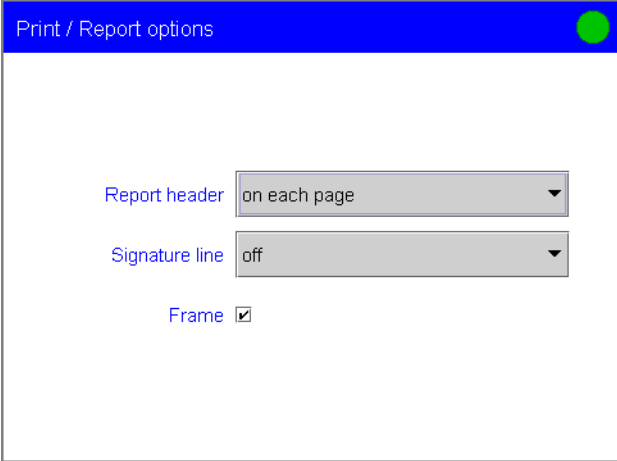
☞ Touch the **[Print]** fixed key.



☞ With **[Print screen dump]** you can activate the "print screen" function. The next time that you touch the **[Print]** fixed key the current screen contents will be printed out.

☞ All upcoming print jobs will be cancelled with **[Clear spooler]**.

☞ Open the dialog for the report configuration with **[Report options]** in the **Print** dialog.



Print / Report options

Report header on each page

Signature line off

Frame

In the Report header the type, serial number and program version of the software (Touch Control or PC Control), the device name which you can enter in the device manager for Touch Control or PC Control, and the printout date with time zone are printed out. You can also define your own report header under **System/Templates/Report header**; this will be printed out in front of the standard report header (see Section 3.14.7).

Under **Report header** you can choose whether the report header is to be printed out on every page, on the first page of the report only or not at all. The **Signature line** gives you the possibility of signing the report together with the date. You can choose whether the **Signature line** is to be printed out on every page, on the first page of the report only or not at all. If the **Frame** checkbox is activated then a frame will be printed round each report page.



Hint!


You can make the sample identifications stand out in the report by printing them in bold print. This is done when they are assigned to a result. Therefore the CALC command must be extended accordingly (see Section 4.5.1).

The following **reports** can be printed out with the **[Print]** fixed key:

	<i>Report</i>	<i>Contents</i>
<i>Print / More reports</i>		
Results (current determination)	Result report	Determination properties, sample data, raw data, i.e. endpoints, final measured values, results of evaluations (EVAL), calculated results, short statistics, messages produced during the determination.
	Curve	The settings for the curve print-out are adopted from the display.
	List of measuring points	List of measuring points
	Calculations	Details of the calculations carried out during the determination sequence (details of every result from the CALC commands, calculated variables and calculated results with the shown accuracy).
	Used devices	All the devices used in the determination sequence as defined under More determination data/Properties .
	Variables	All the determination data; depends on the command.
	Monitoring	Details for the monitored quantities (STAT, DOS only)
Statistics	Statistics short	Summary of the statistics calculations. The number of results, the mean value, absolute and relative standard deviation are printed out for each result.
	Statistics overview	Detailed statistics table, landscape format. The sample data and all individual results are printed out for each determination. The number of results n, the mean value, absolute and relative standard deviation are printed out for each result.
Sample data	Current sample data	Context-sensitive only ; from the main dialog. The sample data is also printed out in the result report.

	<i>Report</i>	<i>Contents</i>
	Sample data silo	Sample data silo properties, landscape format, table with all sample data entered in the sample data silo.
Result table	Result silo	Result silo properties, landscape format, table with all results stored in the result silo.
<i>Print / More reports / Method reports</i>		
Current method	Method sequence	Method properties, list with all method commands.
	Parameters full	Method properties, method options, all method commands with all their parameters. All parameters which no longer have their default settings will be printed out bold . All parameters which have been modified in comparison to the stored version of the method are indicated by an * .
	Titration and measuring parameters	Method properties, all titration and measurement commands with all parameters. All parameters which no longer have their default settings will be printed out bold . All parameters which have been modified in comparison to the stored version of the method are indicated by an * .
	Modified parameters	Method properties, all method commands with parameters which have been modified in comparison to the stored version of the method.
	Non default parameters	Method properties, all method commands with parameters which no longer have the default settings.
<i>Print / More reports / System reports</i>		
System settings	System settings	System settings, settings for acoustic signals and measured value display.
	Dialog options	Dialog options, settings for list of commands and fixed keys, routine dialog settings

	<i>Report</i>	<i>Contents</i>
	User list	Context-sensitive only ; list of all the users defined in the system under user administration. This report can only be printed out by the administrator.
	Login options	Context-sensitive only ; from the edit dialog for login options. List with all login option settings. This report can only be printed out by the administrator.
Titrants	Titrant list	List of all the titrants configured in the system.
	All titrant data short	The most important titrant data for all configured titrants.
	All titrant data full	All titrant data for all configured titrants.
	Titrant data short	Context-sensitive only ; from edit dialog for the titrant. The most important titrant data for the titrant which is currently being edited.
	Titrant data full	Context-sensitive only ; from edit dialog for the titrant. All titrant data for the titrant which is currently being edited.
Sensors	Sensor list	List of all the sensors configured in the system.
	All sensor data short	The most important sensor data for all configured sensors.
	All sensor data full	All sensor data for all configured sensors.
	Sensor data short	Context-sensitive only ; from edit dialog for the sensor. The most important sensor data for the sensor which is currently being edited.
	Sensor data full	Context-sensitive only ; from edit dialog for the sensor. All sensor data for the sensor which is currently being edited.
Device	Device list	List of all devices configured in the system.

	<i>Report</i>	<i>Contents</i>
manager	All device properties	Properties of all the devices configured in the system.
	Device properties	Context-sensitive only ; from edit dialog for the device. Properties of the device which is currently being edited.
GLP manager	GLP data	All data stored in the GLP manager.
Common variables	Common variable list	List of all the common variables defined in the system.
	All common variable properties	Properties of all the common variables defined in the system.
	Common variable properties	Context-sensitive only ; from edit dialog for the common variable. Properties of the common variable which is currently being edited.
Templates	Templates sample data	Sample identification list, sample assignment table.
	Result template list	List of all results templates.
	All results templates details	Details of all results templates.
	Result template details	Context-sensitive only ; from edit dialog for the result template. Details of the result template which is currently being edited.
	Input/Output lines	List of all defined templates for input lines and output lines.
	Custom calibration buffers	Temperature tables for all defined custom calibration buffers.
Rack tables	Rack tables	List of the available racks for the USB Sample Processor with rack name, number of positions and rack code.
Audit trail	Audit trail	Audit trail table (PC Control only). Can also be printed out from the audit trail window with  .

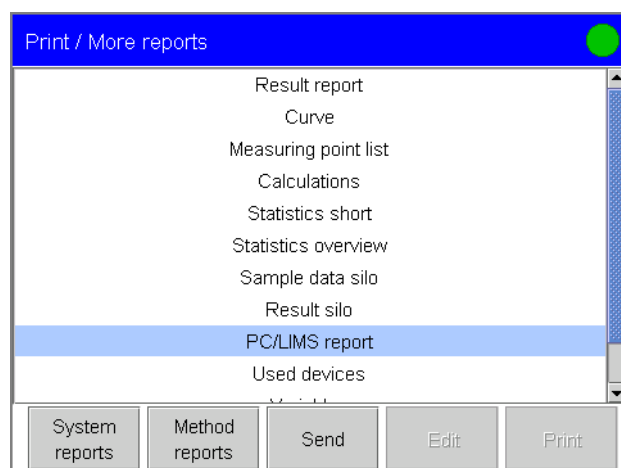
**Note!**

Some tables (statistics overview and sample data silo) are always printed out in **landscape format**, as otherwise the data could not be printed out on a single page. For PC Control you must select the Windows-specific **Printer setting: portrait**, as printout in landscape format is automatic.

3.23.1 Sending or saving a PC/LIMS report

You cannot only automatically send or save a **PC/LIMS report** (ASCII report containing all the most important data of a determination) at the end of a determination (see Section 3.16.10), you can also do this manually with the **[Print]** fixed key. The settings for sending and saving the PC/LIMS report are made in the device manager (see Section 3.10.12). The file name corresponds to the name of the determination which is given by saving the file automatically. A detailed description of the contents of a PC/LIMS report can be found in a separate document, the **Titrande PC/LIMS Report Guide**.

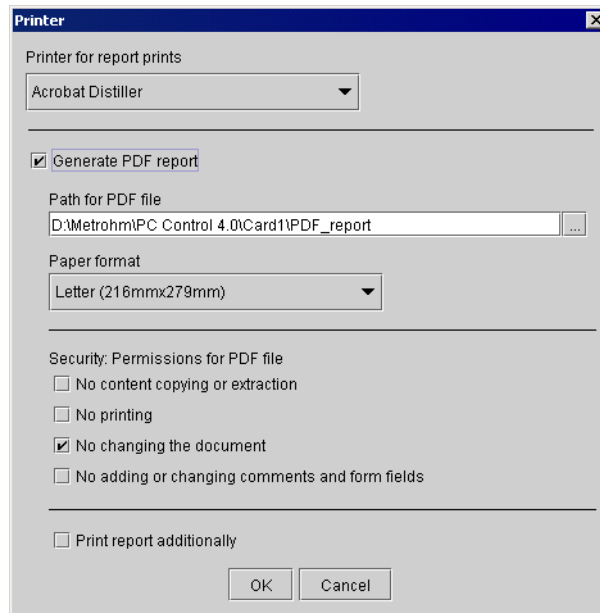
☞ Use the **[Print]** fixed key to open the **Print** dialog and then **[More reports]** to open the list of reports for the current determination.



☞ Select the **PC/LIMS report** in the selection list and send it to the connected PC or save it as a text file with **[Send]**.

3.23.2 Printing PDF reports

☞ Open the edit menu under **File/Printer...**



- **Printer for report prints:** Selecting the printer for the report output on paper from the list of all printers installed on the PC.
- **Generate PDF report:** Activate this checkbox so that you are able to make the following settings for the PDF report.
- **Path for PDF file:** The default setting for the PDF report is a separate folder "PDF_report" in the PC Control installation folder. You can select a different path with [...]. If the report has been printed out with the **[Print]** fixed key then the name of the PDF file corresponds to the report name. The date and time will be appended so that the file name is always unambiguous. For reports that are to be printed out in the method sequence with REPORT command the name corresponds to the determination name.
- **Paper format:** Select the paper format.
- **Security: Permissions for PDF file:** If the checkbox **"No content copying or extraction"** is activated then no copy can be made from the PDF report. If you do not want the report to be printed out then activate the corresponding checkbox. **"No changing the document"** is activated as standard. This means that no alterations can be made. If no comments or form fields are to be added or altered then activate the corresponding checkbox.
- **Print report additionally:** If this checkbox is activated, the report will be printed on the printer selected above additionally to the generated PDF file.

[OK] accepts the settings, **[Cancel]** stops the input without accepting the alterations.

3.24 Manual control

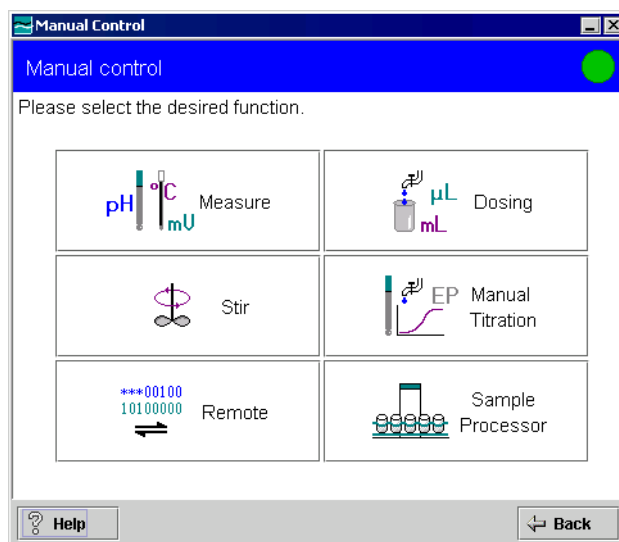
The following functions are available in the manual control:

- Measuring
- Dosing
- Controlling a USB Sample Processor
- Manual titration
- Stirring
- Requesting and setting remote lines

The manual control of devices that are not being used in the sequence is also possible during a determination sequence (BUSY). The dialog for manual control is opened with the **[Manual]** fixed key. With PC Control an additional dialog window is opened so that the PC Control dialog window and the manual control dialog window can be seen side by side.

PC Control:

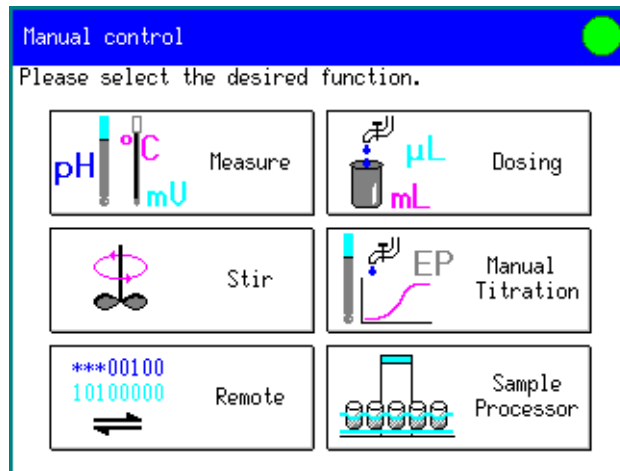
☞ Click on **[Manual]**.



You can open the **online help** for manual control with **[Help]**. In manual control **[Back]** switches to the previous dialog. The Manual control dialog window is closed with **[X]** (close). You can also close the window when a manual run has been started and is not yet finished. In manual control you can recognize when a run has been started by the corresponding symbol in the status line (see *Section 3.6*).

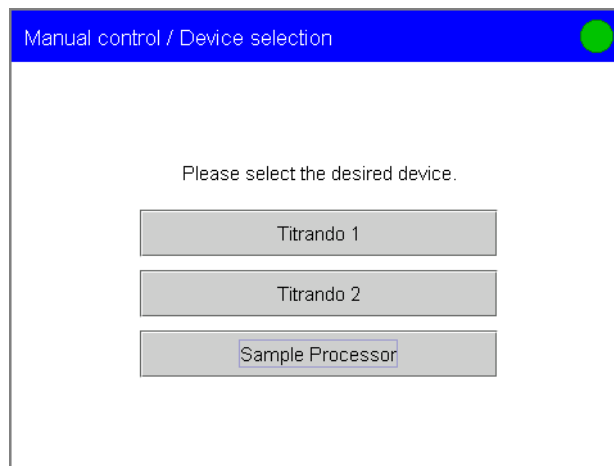
Touch Control:

☞ Touch the **[Manual]** fixed key.



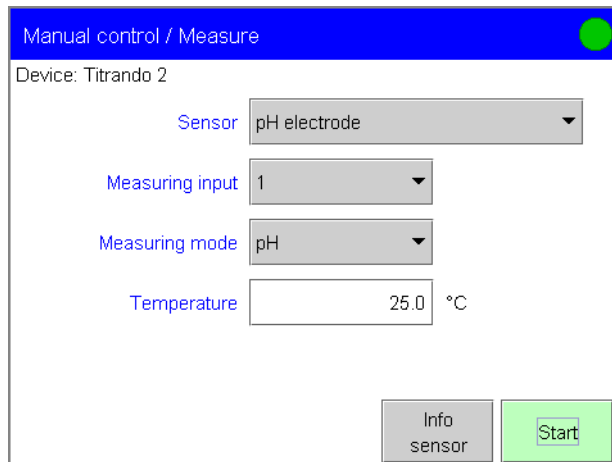
Selecting the control device

If you have connected several control devices then, after selecting the function, possibly you have to select the **control device** (Titrande, USB Sample Processor etc.) that you want to work with. The respective device names are displayed. The name and further settings are configured under **System/Device manager** (see Section 3.10).



3.24.1 Measure

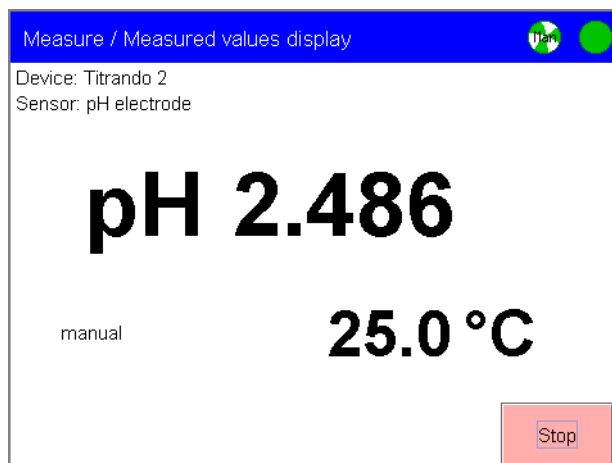
☞ Select the **[Measure]** function in the **Manual control** dialog.



- ☞ First select the **sensor** to be used for the measurement. All the sensors defined under **System/Sensors** will be shown.
- ☞ Select the **Measuring input** to which the sensor is connected.
- ☞ Select the **Measuring mode**. The measuring modes that are suitable for the connected sensor will be shown.
- ☞ If a temperature sensor is connected then the **temperature** will be measured automatically. You can also enter the temperature manually here. This temperature is used for automatic temperature compensation for pH measurements if no temperature sensor is connected. This parameter is not available for the measuring mode **T** (temperature).

The most important sensor data (sensor name, comment, sensor type and, for pH and ISE electrodes, the calibration data) is shown under **[Info sensor]**.

☞ Press **[Start]** to start the measurement. The display switches automatically to the display of measured value.

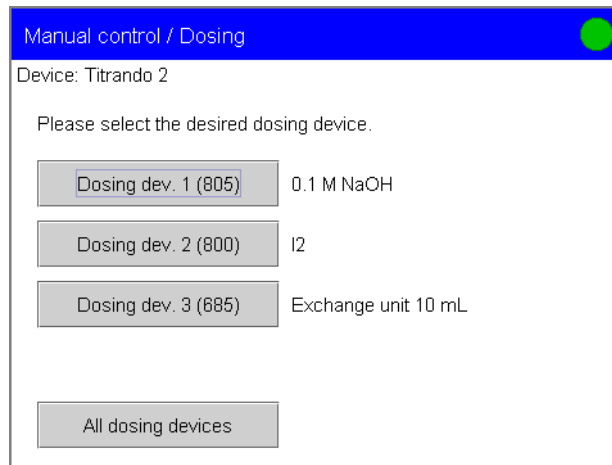


The display of measured value shows the **current measured value**, the type of temperature measurement (**Pt1000**, **NTC** or **manual**) and the **measuring temperature**. The measurement is terminated with **[Stop]**.

3.24.2 Dosing

In the dialog **Manual control/Dosing** you can **dose manually** and **prepare** or **empty** dosing devices. You can also check which dosing devices are connected and which exchange or dosing units are attached.

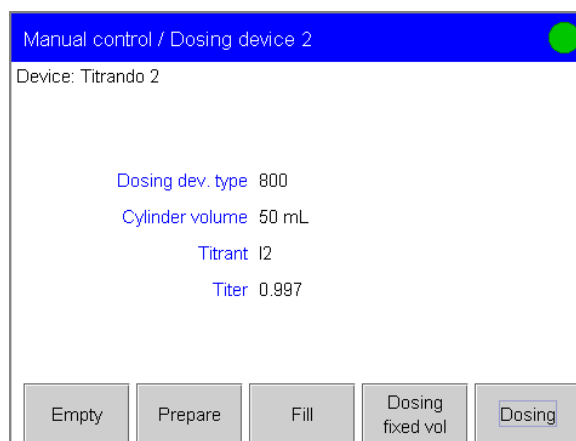
☞ Select the **[Dosing]** function in the **Manual control** dialog. If several dosing devices are connected to a control device then the dialog for selecting a dosing device will be opened. If only one dosing device is connected then the properties of this dosing device will be shown directly:



For every **dosing device** the **connection** (MSB 1 to 4) and the **type** are shown on the button. With type 8XX dosing devices with an intelligent exchange unit or dosing unit the **titrant** will be shown to the right. With type 6XX or 7XX dosing devices only the cylinder volume of the exchange or dosing unit will be shown. If the exchange or dosing unit is not (correctly) attached to a connected dosing device then "----" will be shown. If a dosing device is busy with the determination sequence then this will be indicated accordingly with "Manual busy".

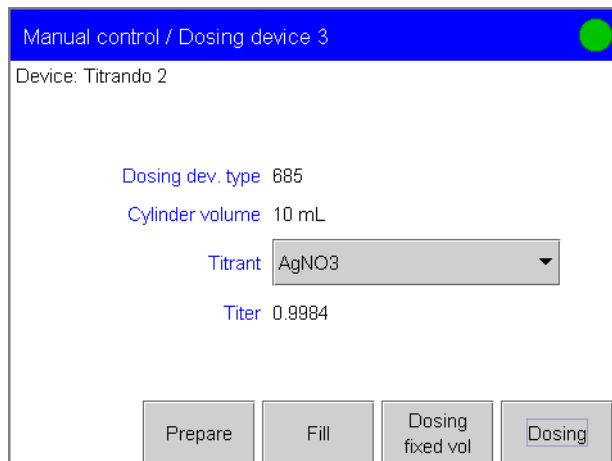
With **[All dosing devices]** you can carry out the commands **Fill**, **Prepare** and **Empty** for several dosing devices of a control device at the same time.

☞ Select the **dosing device** to be controlled manually.



For type 8XX dosing devices with an intelligent exchange unit or dosing unit the data stored on the data chip will be displayed.

For type 6xx or 7xx dosing devices you can select a titrant from the titrants configured under **System/Titrants**. Only those titrants which are suitable for use with the corresponding type of dosing device will be shown in the selection list, i.e. dosing units for Dosinos and exchange units for Dosimats. The cylinder volume is checked when dosing is carried out.

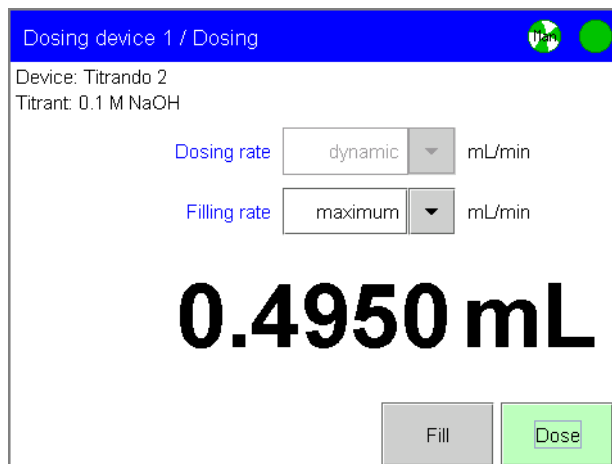


The details of the subdialogs are described on the following pages.

Dosing

Under manual control dosing will be carried out for as long as the **[Dose]** button is pressed down.

☞ Press **[Dosing]** to open the dialog for manual dosing.



☞ Enter the **Dosing rate**. The rate should be reduced for viscous liquids. The maximum dosing rate depends on the cylinder volume of the exchange or dosing unit used (see *Section 3.8.6*). **Dynamic** means that dosing will be carried out quicker and quicker until the maximum dosing rate has been reached (starting with 1 mL/min and then doubling the dosing rate every 1.5 s). **Dynamic** can only be selected when the dosing cylinder is filled. If dynamic dosing is

selected then the dosing rate cannot be altered while dosing is taking place.

- ☞ Enter the **Filling rate**. The rate should be reduced for viscous liquids. The maximum filling rate depends on the cylinder volume of the exchange or dosing unit used (see *Section 3.8.6*).
- ☞ You can carry out manual dosing with **[Dose]**. When a cylinder volume has been added, the dosing cylinder will be refilled automatically.
- ☞ You can refill the dosing cylinder with **[Fill]**. The shown volume will be reset to 0.0000 mL.

If you exit the dialog with **[Back]** then the dosing cylinder will be refilled automatically and the valve switched to the exchange position.

Dosing fixed volume

Under **Dosing device/Dosing fixed volume** you can add a specified volume.

- ☞ Open the dialog with **[Dosing fixed volume]**.

Dosing device 1 / Dosing fixed volume

Device: Titrand 2
Titrant: 0.1 M NaOH

Volume mL

Dosing rate mL/min

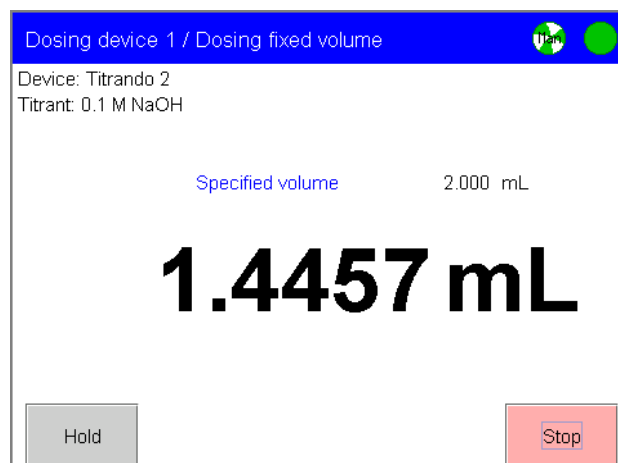
Filling rate mL/min

Fill automatic

- ☞ Enter the desired volume.
- ☞ Enter the **Dosing rate**. The rate should be reduced for viscous liquids. The maximum dosing rate depends on the cylinder volume of the exchange or dosing unit used (see *Section 3.8.6*).
- ☞ Enter the **Filling rate**. The rate should be reduced for viscous liquids. The maximum filling rate depends on the cylinder volume of the exchange or dosing unit used (see *Section 3.8.6*).

If the **Fill automatically** checkbox is activated then the dosing cylinder will be refilled automatically after dosing has been carried out and the added volume will be reset to 0.0000 mL in the volume display (see below). If you want to carry out successive dosing cycles and if the volumes that are already dosed are to be accumulated then deactivate the checkbox. The added volume will only be reset to 0.0000 mL when the dosing cylinder is refilled with **[Fill]**.

- ☞ Press **[Start]** to start the addition of the preset volume. The display switches automatically to the volume display.



The specified volume is shown above the volume that is already dosed. If the **Fill automatically** checkbox is deactivated then the button **[Fill]** is available additionally.

[Stop] is used to stop the addition. You can use **[Hold]** to interrupt the addition and continue it with **[Continue]**.

Fill

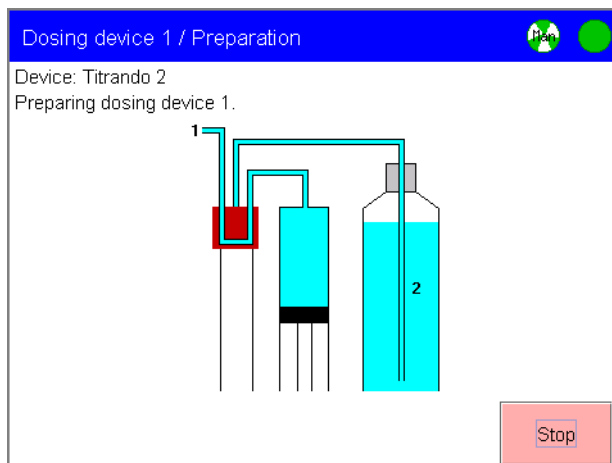
You can fill the dosing cylinder manually with the **[Fill]** function. The piston and valve positions are shown during the filling process. Filling is carried out at the maximum filling rate.

Prepare

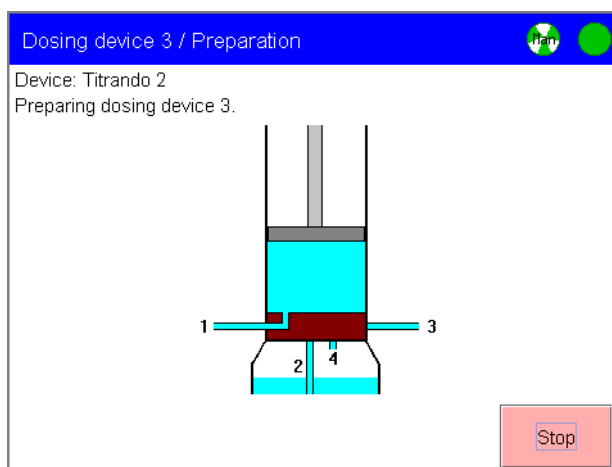
The **[Prepare]** function is used to rinse the cylinder and tubing of the exchange unit or dosing unit and to fill bubble-free. You should carry out this function before the first determination or once per day.

The parameters defined for the titrant under **System/Titrants** for preparing the exchange or dosing unit and the tubing parameters will be used for rinsing (see *Section 3.8.6*). For every dosing device you can define in the **Device manager** when a message is to be shown to remind you that the dosing device has to be prepared (see *Section 3.10*).

☞ Start the preparation process with **[Prepare]**. The display switches automatically to the live display.



Example: Exchange unit



Example: Dosing unit

Empty

The **[Empty]** function can only be carried out with dosing units. The Empty function empties the cylinder and all the tubing of the dosing unit. The parameters defined under **System/Titrants** for preparing the dosing unit and the tubing parameters are used for emptying (see *Section 3.8.6*).

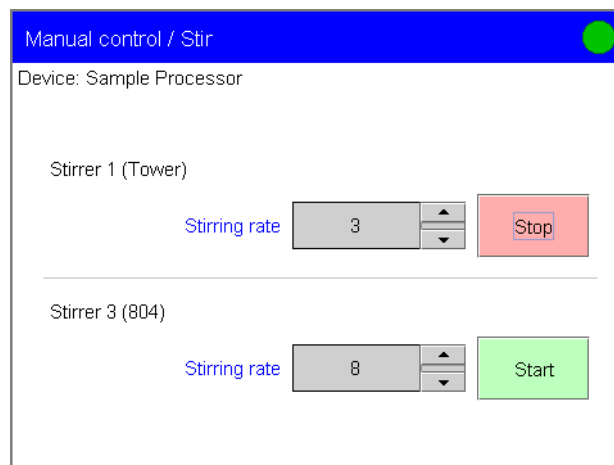
You can use the empty and prepare functions to change easily the reagent of a dosing unit without coming into contact with chemicals. Proceed as follows:

- ☞ Empty the dosing unit with **[Empty]**.
- ☞ Carry out the **[Prepare]** function using a suitable solvent to rinse the dosing unit.
- ☞ Empty the dosing unit with **[Empty]**.
- ☞ Carry out the **[Prepare]** function using the new reagent.

3.24.3 Stir

All the connected stirrers can be controlled manually.

☞ Select the **[Stir]** function in the **Manual control** dialog.



The **connection** (MSB 1...4) and (in brackets) the **stirrer type** are shown for each **Stirrer**.

☞ You can increase the stirring rate with **[↑]** or **[+]** and decrease it with **[↓]** or **[-]**. The stirring direction changes as the sign changes ("+" means counterclockwise and "-" means clockwise when seen from above). The stirring rate can also be altered while the stirrer is running. The default setting **8** corresponds to 1000 rpm (see *Section 4.1.5, Fig. 4.14*).

☞ **[Start]** starts stirring and **[Stop]** stops it.

If you have connected more than two stirrers then you can open the dialog for the additional stirrers with **[More stirrers]**.

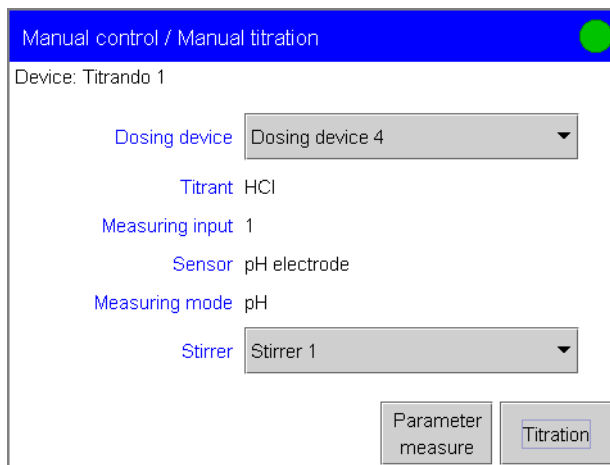
If you have started a stirrer manually then it will not be switched off automatically at the start of a determination. This means, for example, that you can switch on the stirrer before the start of a determination in order to dissolve the sample. The stirrer will continue to run during the determination until it is switched off in the determination sequence.

If a stirrer is used in the determination sequence it can nevertheless be controlled manually at the same time. You can, for example, use the manual control to reduce the stirring rate of a stirrer which has been started in the determination sequence.

3.24.4 Manual titration

Manual titrations can be carried out in the pH, U (mV), I_{pol} (mV), U_{pol} (μA), concentration and T (°C) measuring modes.

☞ Select the **[Manual titration]** function in the **Manual control** dialog.



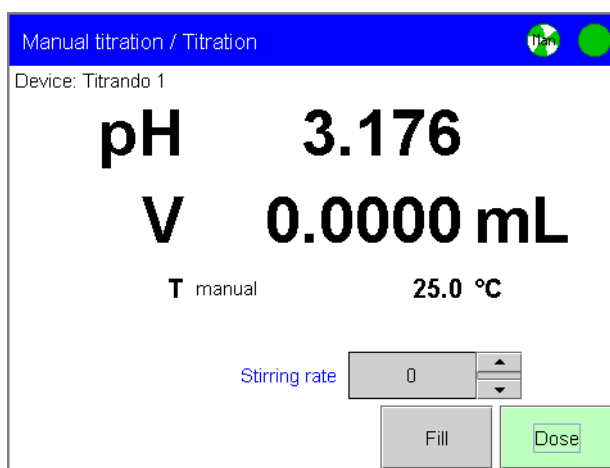
☞ Select a **Dosing device**. With intelligent exchange or dosing units the **Titrant** contained in the exchange or dosing unit will be displayed. With "non-intelligent" units the cylinder volume will be shown.

☞ Select a **Stirrer**.

You can choose the measuring input, sensor and measuring mode under **[Parameter measure]**.

☞ Use **[Parameter measure]** to open the edit dialog for the measuring parameters and enter these.

☞ Use **[Titration]** to open the live dialog for the manual titration.



The live dialog shows the **current measured value**, the added **volume**, the type of temperature measurement (**Pt1000**, **NTC** or **manual**) and the **measured temperature**.

☞ You can increase the stirring rate with **[↑]** or **[+]** and decrease it with **[↓]** or **[-]**. The stirring direction changes as the sign changes

("+" means counterclockwise and "-" means clockwise when seen from above).

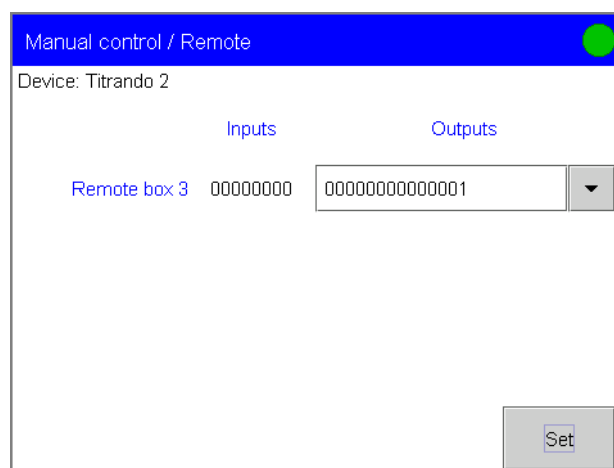
- ☞ You can carry out manual dosing with **[Dose]**. The dosing cylinder will be refilled automatically when a cylinder volume has been added. Dosing will be carried out for as long as long as the **[Dose]** button is pressed down. The addition is always **dynamic**, i.e. dosing will be carried out quicker and quicker until the maximum dosing rate has been reached (starting with 1 mL/min and then doubling the dosing rate every 1.5 s).
- ☞ Read the added volume.
- ☞ You can refill the dosing cylinder with **[Fill]**. The shown volume will be reset to 0.0000 mL.

If you exit the dialog with **[Back]** then the dosing cylinder will be refilled automatically and the valve switched to the exchange position.

3.24.5 Remote

At the remote box you can **set output lines** manually. The status of the **input lines** is scanned automatically.

- ☞ Select the **[Remote]** function in the **Manual control** dialog.



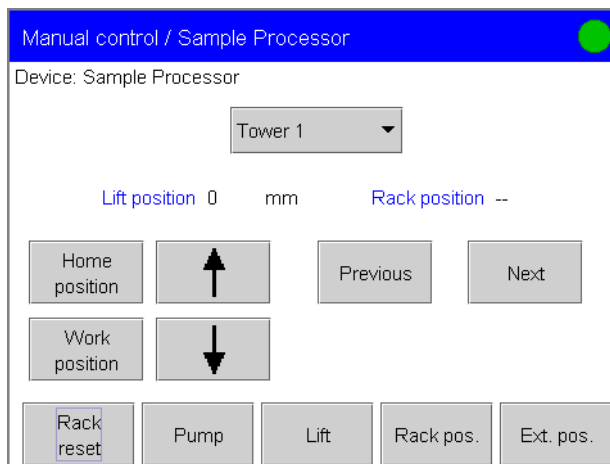
The current status of the input lines will be shown for each connected remote box. The output lines can be set. The input and output lines are always numbered from right to left starting with 0. Consequently, the output line 0 is set with the signal "0000000000000001". Please consult the **online help** for entering the binary pattern. You can select binary patterns defined in the selection list under **System/Templates**.

- ☞ The binary patterns defined under Outputs are set with **[Set]**.

3.24.6 USB Sample Processor

With a connected **USB Sample Processor** you can trigger any movement or function manually. You can end lift and rack movements prematurely with **[Stop]**.

☞ In the dialog **Manual control** select the function **[Sample Processor]**.



☞ **[Rack reset]** must be pressed if you have positioned a new rack or have carried out alterations to the current rack table in the device manager without having them transferred directly afterwards to the USB Sample Processor (see Section 3.10.5). The lift and rack are then moved to the zero position, the rack code is read off and the corresponding rack data is transmitted to the USB Sample Processor. The USB Sample Processor is now not at a valid rack position, this is indicated under **Rack position** by "--". This rack reset corresponds to the method command RACK or the method start option **Rack reset**.

☞ If you have connected a USB Sample Processor equipped with 2 towers then you must first select the tower to be used for the following manual operation: **Tower 1** or **Tower 2**. When viewed from the front **Tower 1** is at the **right** and **Tower 2** at the **left**.

Lift position and **Rack position** give the current position of the lift and rack at any time for the selected tower. After a new start or a rack reset the rack is at the zero position. This is indicated with "--".



Note!

Please remember that for all the following lift movements a valid current rack position must be indicated! Otherwise a corresponding error message will appear. Carry out a MOVE command or move to a valid rack position with **[Previous]** or **[Next]**.

☞ **[Home position]** moves the lift to the 0 mm position, i.e. to the uppermost stop.

☞ **[Work position]** moves the lift to the previously defined work position. This is defined in the rack table (see Section 3.10.5) of the current rack or can be assigned directly under **[Lift]** (see below).

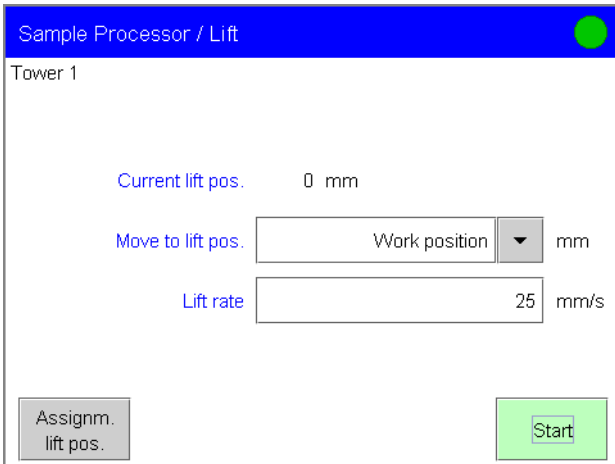
- ☞ The two arrows **[↑]** and **[↓]** can be used to move the lift directly up and down for as long as the button is kept pressed down. The current lift position is shown continuously.
- ☞ **[Previous]** and **[Next]** rotates the previous or next rack position such that it is placed in front of the selected tower or robotic arm.

Pump

- ☞ Activate **[Pump]** in order to access the control of the pumps. You can now turn the pumps on and off. Two pumps that can be controlled are always shown for each tower. Two connections for external pumps are available if no pumps are installed.

Lift

- ☞ With **[Lift]** you can access the control of the lift.



Sample Processor / Lift

Tower 1

Current lift pos. 0 mm

Move to lift pos. mm

Lift rate mm/s

Assignm. lift pos.

- ☞ Select the predefined lift positions under **Move to lift pos.** or enter the required lift position and press **[Start]**. The lift is moved to the required position.

The rate defined under **Lift rate** is only valid for manual control. A separate lift rate can be defined in the command LIFT for automatic operation.

The predefined lift positions are specified in the Device manager in the current rack table (see *Section 3.10.5*). They can also be assigned directly here:

- ☞ Move the lift to the position that you want to set as a new predefined lift position. Either use the **[↑]** and **[↓]** buttons or enter the required lift position in mm in the subdialog **Lift** and press **[Start]**.
- ☞ With **[Assignm. lift pos.]** you can access the predefined lift positions that you can now assign to the current lift position. Depending on the current rack position, each lift position that can be set is now available:

General rack position (not an external position, not a special beaker):

A work position, a shift position, a rinse position and a special position can be defined for general rack positions.

Lift / Assignment lift position ●

Current lift pos. 50 mm

Position name	Position height
Work position	130 mm
Shift position	50 mm
Rinse position	100 mm
Special position	0 mm

Special beaker:

An individual specific work position can be defined for each special beaker. The shift, rinse and special position of the affected tower are taken from the general rack positions.

Lift / Assignment lift position ●

Current lift pos. 130 mm

Position name	Position height
Work position	130 mm
Shift position	--
Rinse position	--
Special position	--

External position (with Swing Head only):

With the external positions a specific work position can be defined for each of the four positions. A shift and rinse position can only be defined for all four external positions together. No special position can be assigned here.

Lift / Assignment lift position ●

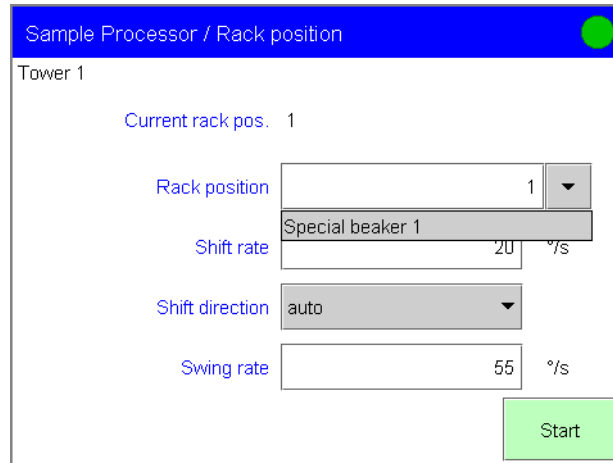
Current lift pos. 70 mm

Position name	Position height
Work position	110 mm
Shift position	35 mm
Rinse position	70 mm
Special position	--

☞ Select the required lift position and press **[Assign]**.

Move to rack position

☞ **[Rack pos.]** accesses the selection of the special beaker positions.



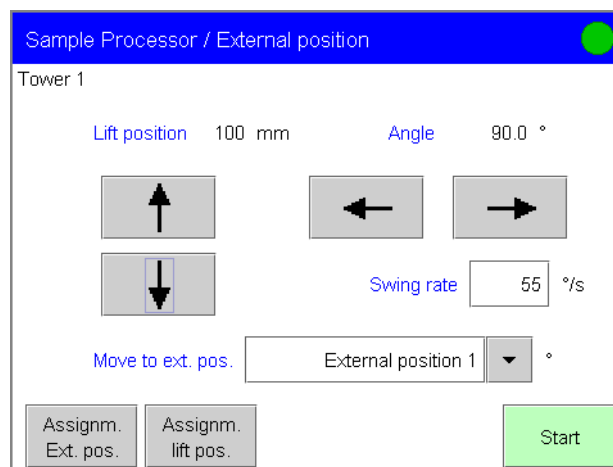
☞ Select the required entry under **Rack position** or enter an absolute rack position and press **[Start]**. The required rack position is moved to.

Only those special beakers will be offered for selection that are defined in the current rack table (see Section 3.10.5).

The **shift rate** and the **shift direction** of the sample rack can be changed here. If the option "auto" is selected as shift direction, then the sample rack rotates automatically in the direction in order to result in the shorter way. "+" means that the direction of rotation is always counterclockwise and "-" means that the direction is always clockwise. The **swing rate** is the speed of the robotic arm.

External positions

☞ With **[Ext. pos.]** you access the selection of the 4 external positions.



- ☞ The [**←**] and [**→**] arrows move the robotic arm to the left or to the right, respectively. As soon as you release the arrow key the current angle position will be shown.
- ☞ With [**Assignm. Ext. pos.**] you can now assign a swing angle to the individual external positions.
- ☞ Under **Move to ext. pos.** you can select the required external position directly or you can also enter a swing angle. Pressing [**Start**] moves to the corresponding angle position.

The buttons for setting the lift position only become active when the robotic arm is moved to an external position with [**Start**]. You can move the lift to the required lift position with the [**↑**] and [**↓**] keys. With [**Assignm. lift pos.**] you can assign a work position to each of the individual external positions and also assign a shift and rinse position for all four external positions together. These settings can also be made in the properties of the Swing Head (see *Section 3.10.5*). When moving to an external position or a certain angle by pressing [**Start**] you can define the speed of the robotic arm with **Swing rate**.

4 Parameters

All the **parameters for the method commands**, from which a list of commands can be constructed, are explained in this section. How you can insert an individual command in the list of commands is described in *Section 3.16.2*. The way of selecting a command from the list and editing it is described in *Section 3.16.1*.

With many numerical inputs you can also enter a **special value** (e. g. **off**) or a **result** that has previously been calculated (e. g. **R1**) instead of a number. With PC Control you can enter the special value with the arrow to the right of the input field. The result variables are entered directly via the PC keyboard. Numerical input for Touch Control is described in *Section 3.1.4*.

Parameters which are available as direct parameters (see *Section 3.16.5*) are marked with (d). For further **details about individual parameters**, e. g. the **input range and default values**, please use the context-sensitive **online help** (see *Section 3.3.3*).

The titration, measuring and calibration commands as well as the evaluations cannot be carried out with the 846 Dosing Interface because this device doesn't have a measuring interface.

An overview of the devices and their titration and measurement modes can be found in the appendix in *Section 6.6*.

4.1 Titrations

The following titration modes are available:

- **Dynamic equivalence point titrations (DET)** with dynamic incremental reagent addition for all standard titrations. The volume increments vary as a function of the slope of the curve. An attempt is made to achieve constant measured value alterations with each reagent addition. The optimal volume for dosing is determined from the measured value alterations of the previous reagent additions. Measured value acceptance is drift-controlled (equilibrium titration) or after a waiting period. Equivalence points are evaluated automatically.

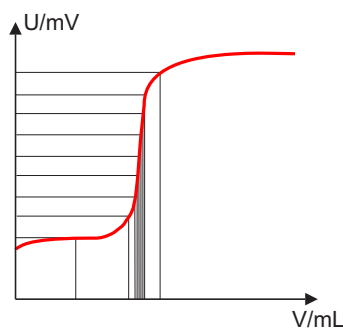


Fig. 4.1: Reagent addition for DET

**Note!**

As the reagent addition in DET depends on the measuring data, the titration curve should not vary too much from an **S-shaped curve**.

- **Monotonic equivalence point titrations (MET)** with reagent addition at constant volume increments for titrations with relatively high signal variations or suddenly occurring potential jump and for slow titrations or slowly responding electrodes. Measured value acceptance is drift-controlled (equilibrium titration) or after a waiting period. Equivalence points are evaluated automatically.

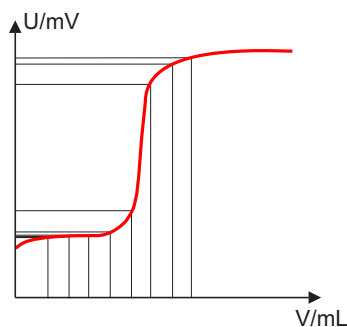


Fig. 4.2: Reagent addition for MET

- **Endpoint titrations (SET)** for rapid routine determinations by titration to a preset endpoint (e. g. titrations according to special standards) and titrations in which an excess of reagent must be avoided. The termination of the titration at the endpoint is either drift-controlled or after a waiting period. The volume that has been added when the endpoint is reached gives the calculable reagent consumption.

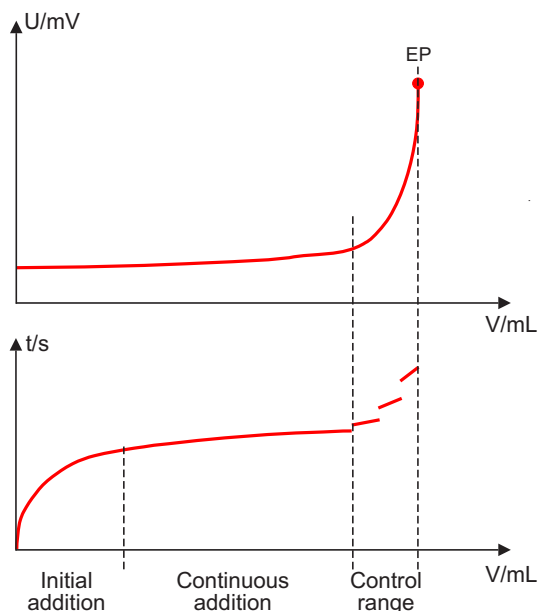


Fig. 4.3: Reagent addition for SET

- Karl Fischer titration (KFT)** for determining the water content by the Karl Fischer method with automatic pre- and post-conditioning. A typical feature of the Karl Fischer titration is the controlled reagent addition, which depends on the control difference (current measured value – endpoint), with the aim of reaching the measured value given as being the predefined target endpoint as quickly and accurately as possible. Overtitrating is avoided to a great extent. The titration termination at the endpoint takes place either drift-controlled or after a waiting period. The volume added up to the endpoint gives the calculable reagent consumption.

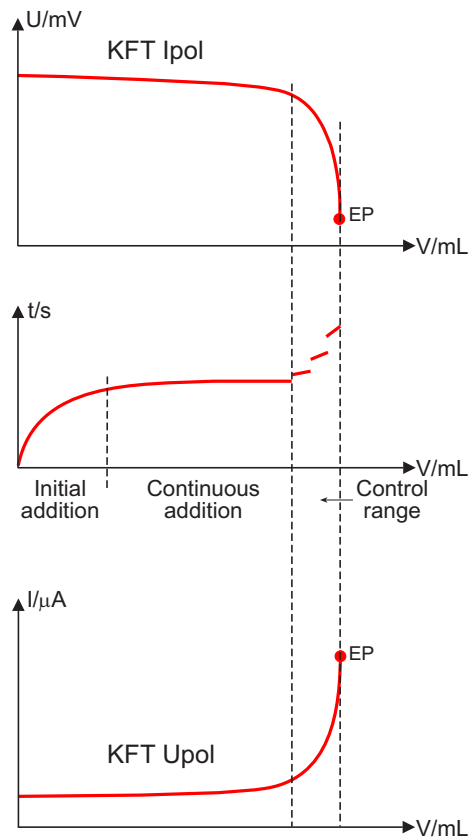


Fig. 4.4: Reagent addition for KFT

The **measuring modes** pH (potentiometric pH measurement), U (potentiometric voltage measurement), I_{pol} (voltametric measurement with selectable polarization current) and U_{pol} (amperometric measurement with selectable polarization voltage) can be selected for all titrations.

- **Endpoint titrations while holding the measured value constant.** pH STAT is the most frequently used titration. A reagent is used to dose to a preset measured value (control point). This control point is kept constant by titrating the reaction product continuously with the reagent. The STAT titration keeps the control point constant until the preset stop condition has been reached. The STAT titration is used, for example, in enzymatic analysis. The dosing rate resulting from holding the control point constant provides information about enzyme activity.

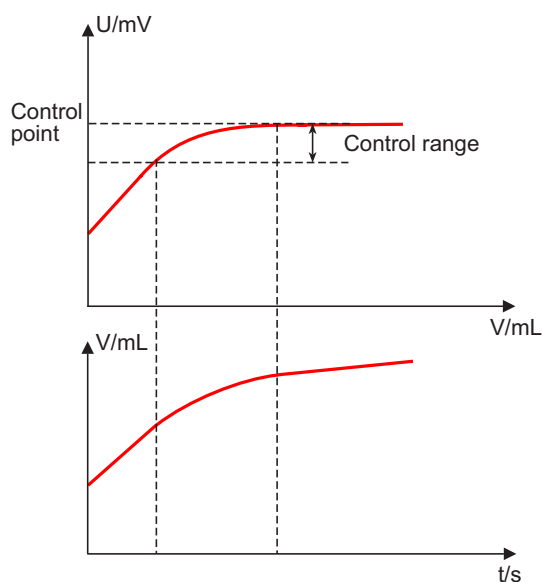


Fig. 4.5: Reagent addition for STAT

pH and U are the only **measuring modes** that are available for the STAT titration.

4.1.1 Dynamic equivalence point titrations (DET) and monotonic equivalence point titrations (MET)

For equivalence point titrations (DET, MET) the parameters are identical except for a few exceptions. Both modes are described together here.

Start conditions

Under **Start conditions** the parameters for the initial addition of titrant and for the initial measured value (measured value before start conditions are processed) can be edited:

- **Start volume** (d): Volume which is added before the start of the titration. Under **Dosing rate** (d) you can enter the rate at which the start volume is added.
- **Pause** (d): Waiting period which is to elapse before the start of the titration after the start conditions have been fulfilled.
- **Start measured value** (d): Measured value at which the initial dosing is stopped. Under **Dosing rate** (d) you can enter the rate to be used until the start measured value or the start slope have been reached.
- **Start slope** (d): Slope (measured value per unit volume) at which the initial dosing is stopped. Under **Dosing rate** (d) you can enter the rate to be used until the start measured value or the start slope has been reached.

The start conditions are processed in succession: 1. Start volume, 2. Start measured value, 3. Start slope, 4. Pause.

Parameters for the **Initial measured value**:

- **Signal drift** (d): Drift, i.e. the alteration in the measured value per minute, which has to be reached before the measured value will be accepted.
- **Waiting time min.** (d): The measured value is not accepted until the minimum waiting time has elapsed, even if the measured value drift has already been reached. The minimum waiting time is only important for drift-controlled measurements.
- **Waiting time max.** (d): If the signal drift is switched off or has not yet been reached then the measured value will be accepted after the maximum waiting time has elapsed.

Titration parameters

Under **Titration parameters** you can edit the parameters for the titration procedure:

- **Titration rate** (d): Three predefined sets of parameters can be selected for the titration rate (see Table on p. 199). If individual titration parameters need to be adapted you should select the setting **User** and edit the individual titration parameters under **User-defined Parameters**.
- **Temperature** (d): Manually entered titration temperature. If a temperature sensor is connected and the temperature measurement is set to **automatic** or **continuous** under **Sensor** (see Section 4.1.5) then the temperature will be measured continuously. The value is used for temperature compensation in pH measurements.

The **User-defined Parameters** differ for dynamic equivalence point titrations (DET) and monotonic equivalence point titrations (MET).

User-defined titration parameters for DET and MET

- **DET: Measuring point density** (d): A small value means small volume increments, i.e. a high measuring point density. The curve then shows all the finest details which also include noise; this could cause unwanted equivalence points to be found. A larger value, i.e. a smaller measuring point density, permits quicker titrations. If you are using a dosing device with a small cylinder volume then a smaller measuring point density value may be beneficial. However, you should also set a smaller measured value drift and a higher EP criterion at the same time.
- **DET: Minimum (volume) increment** (d): This smallest permitted volume increment is added at the start of the titration and with steep curves in the equivalence point region. Very small values should only be used if a low titrant consumption is expected, as unwanted equivalence points could be evaluated.



Note!

It is not advisable to select similar volumes for the minimum and maximum increments. For these applications monotonic equivalence point titration (MET) is more suitable.

- **DET: Maximum (volume) increment** (d): A maximum volume increment should be selected when the titrant consumption up to the equivalence point is expected to be very small, a start volume is to be added until just before the equivalence point is reached or if the change of direction in the potential jump region is very abrupt, as otherwise it is easy to add too large a volume in the equivalence point region. The value should not be less than 1/100 cylinder volume.
- **MET: Volume increment** (d): Volume to be added at each dosing step. The choice of the correct volume increment is a basic requirement for achieving high accuracy. A good guideline is 1/20 of the expected EP volume. For steep jumps the volume increment should tend toward 1/100 and for flat jumps toward 1/10 of the EP volume. Small volume increments are used for determining blank values or with very asymmetrical curves. The accuracy of the evaluation cannot be increased by using smaller increments as the measured value alterations between two measuring points are then of the same order of magnitude as the noise.
- **Dosing rate** (d): Rate at which the volume increment is added. The maximum dosing rate depends on the cylinder volume of the exchange or dosing unit used (see Section 3.8.6).
- **Signal drift** (d): Drift, i.e. the alteration in the measured value per minute that has to be reached for measured value acceptance. This type of titration is often known as an equilibrium titration. **off** means that the measured value acceptance takes place when the maximum waiting time has elapsed. This may be advisable if the titration reaction occurs slowly or if the electrode has a slow response.



Note!

A **constant measured value** is often only achieved after a certain time, as mixing and possibly the reaction itself require a certain time. The response time of an electrode can also increase with time, i.e. reaching a constant measured value takes longer and longer. In such a case **drift-controlled measured value acceptance** is particularly advisable, as the measured values are only accepted when equilibrium has almost been achieved.

- **Waiting time min. (d):** The measured value is not accepted until the minimum waiting time has elapsed, even if the measured value drift has already been reached. The minimum waiting time is only important for drift-controlled measurements.
- **Waiting time max. (d):** If the signal drift is switched off or has not yet been reached then the measured value will be accepted after the maximum waiting time has elapsed. If the waiting time has not been newly entered then a waiting time that is suitable for the drift will be calculated automatically according to the following equation:

$$\text{Waiting time} = 150/\sqrt{\text{Drift} + 0.01} + 5$$



Note!

Select **titration rate optimal** when you are developing a **new titration method**. This parameter is suitable for virtually all titrations and only needs adaptation in special cases.

Parameters for predefined titration rates for DET and MET

	Titration rate	slow	optimal	fast
DET	Meas. point density	2	4	6
	Min. vol. increment	10.00 µL	10.00 µL	30.00 µL
	Max. vol. increment	off	off	off
MET	Volume increment	0.05000 mL	0.10000 mL	0.20000 mL
DET and MET	Dosing rate	maximum	maximum	maximum
	Measured value drift	20.0 mV/min 20.0 µA/min	50.0 mV/min 50.0 µA/min	80.0 mV/min 80.0 µA/min
	Waiting time min.	0 s	0 s	0 s
	Waiting time max.	38 s	26 s	21 s

Stop conditions

The conditions for terminating the titration are defined under **Stop conditions**:

- **Stop volume** (d): Stops when the preset volume (including start volume) has been added since the start of the titration. The stop volume should be adapted to suit the sample weight or the titration vessel size.
- **Stop measured value** (d): Stops when the preset value for a measuring point has been exceeded or undercut since the start of the titration.
- **Stop EP** (d): Stops when the preset number of equivalence points has been found.
- **Volume after EP** (d): When the number of equivalence points defined under **Stop EP** has been found this volume will be added. In this way the curve can be continued after the equivalence point has been reached.
- **Stop time** (d): Stops when the preset time (including start conditions) has elapsed since the start of the titration.

If several stop conditions have been set then the first criterion to be fulfilled will stop the titration.

- **Filling rate** (d): Rate at which the dosing cylinder is refilled after the titration. The maximum filling rate depends on the cylinder volume of the exchange or dosing unit used (see *Section 3.8.6*).

Pot. evaluation

Under **Potentiometric evaluation** the parameters for the evaluation of the titration curve, i.e. for automatic equivalence point recognition, are edited:

- **EP criterion** (d): The set equivalence point criterion is compared with the ERC (**E**quivalence point **R**ecognition **C**riterion) which has been found. Equivalence points whose ERC is smaller than the set EP criterion will not be recognized (see *p. 203* and *p. 204*). The default value is suitable for most titrations.
- **EP recognition** (d): This parameter allows you to filter out the endpoints you are looking for. Either **all** the equivalence points can be recognized, or only those which meet particular criteria: the **greatest** (only the EP with the largest ERC, i.e. the steepest jump), the **last** (only the last EP to be found), **ascending** (only EPs with a positive titration curve slope), **descending** (only EPs with a negative titration curve slope).
- **Set windows**: Up to nine ranges (windows) can be defined on both the measured value axis as well as on the volume axis. Only equivalence points in the preset windows will be recognized and numbered according to the window (e. g. EP2 in window 2).

A window defines a range in which an equivalence point is expected. Equivalence points outside this range will not be recognized. Setting windows is advisable when interference and unnecessary equivalence points are to be suppressed. The list of windows is opened with **[Set windows]**.

Pot. evaluation / Set windows

01 DET pH Dynamic pH titration

No.	Lower limit	Upper limit
1	pH 2.000	pH 3.000
2	pH 5.000	pH 6.000

New Delete Edit

When the list is opened for the first time you will see that it already contains a window which covers the whole measured value or volume range. You can add and edit new windows with **[New]**. The selected window can be removed from the list with **[Delete]**. You can use **[Edit]** to adapt the upper and lower limits for the selected window. All calculable variables can also be applied as result variable R1...R9. This means that you have to define the results in a preceding CALC command. If results are used as limits, only one window can be set then. Windows must not overlap but may touch one another. Equivalence point recognition criteria can be defined for each window. Please note that no direct parameters can be defined for setting windows.

Set windows / Edit

02 DET pH Dynamic pH titration

Lower limit mL

Upper limit mL

EP criterion

EP recognition

- **Lower limit:** Measured value or volume for the lower limit of the window.
- **Upper limit:** Measured value or volume for the upper limit of the window.
- **EP criterion:** The set equivalence point criterion is compared with the ERC (**E**quivalence point **R**ecognition **C**riterion) which has been found. Equivalence points whose ERC is smaller than the set EP criterion will not be recognized (see below). The default value is suitable for most titrations.
- **EP recognition:** Only equivalence points which fulfill particular criteria will be recognized: the **first** (only the first EP to be found), the **greatest** (only the EP with the largest ERC, i.e. the steepest jump),

the **last** (only the last EP to be found), **ascending** (only EPs with a positive titration curve slope), **descending** (only EPs with a negative titration curve slope).

Only one equivalence point will be recognized per window. The numbering of the equivalence point (EP) is determined by the numbering of the window (e. g. EP2 in window 2), so that even if EPs are missing the calculations will still be carried out with the correctly assigned EP volumes.

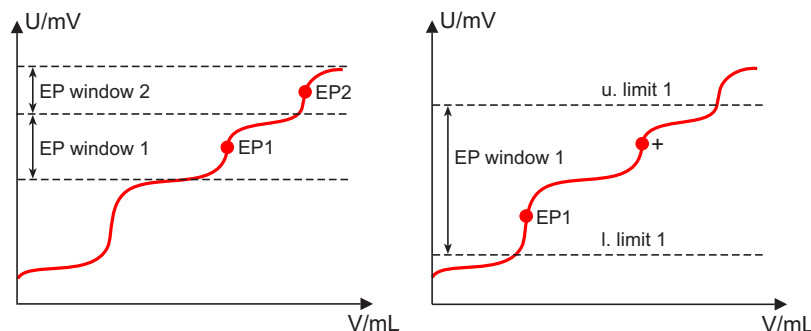


Fig. 4.6: Equivalence point recognition and numbering in windows

In the first example in Fig. 4.6 two equivalence points have been recognized in two different windows (EP1 in window 1 and EP2 in window 2). In the second example two equivalence points have been recognized in a single window, but only the first one will be recognized and the second jump will not. In order that the user can recognize that more than one equivalence point has been found in the set window, EP1 is marked with a '+' in the result display. In addition, the message **Several EPs in the window** will be entered in the list of messages.

The **evaluation of the titration curve** and therefore the EP criterion for the recognition of the equivalence points is different for dynamic equivalence point titrations (DET) and monotonic equivalence point titrations (MET).

Evaluation and equivalence point criterion in the DET mode

Equivalence points (EPs) are determined in a similar manner to that described in the Tubbs method (C.F. Tubbs; Anal. Chem 26 (1954) 1670–1671, quoted in Ullman 5 (1980) 659). The volume of the equivalence point (V_E) is shifted from the point of inflection towards the smaller circle of curvature for real asymmetric titration curves.

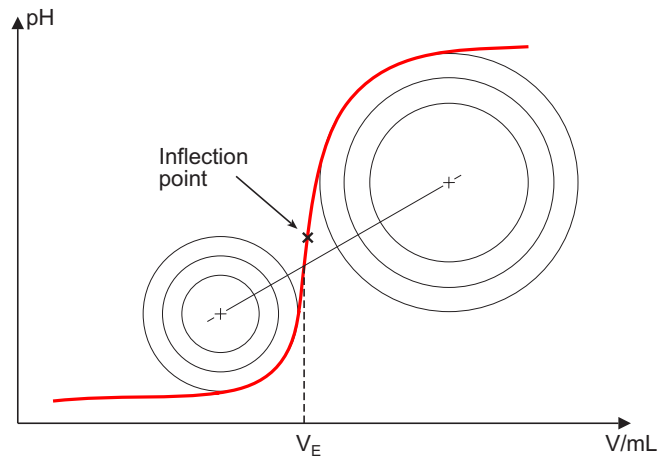


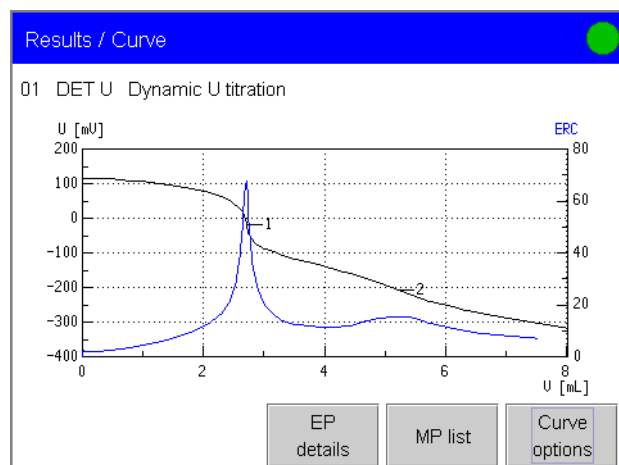
Fig. 4.7: Tubbs method for determining the equivalence point

The figures shows that the evaluation also requires measuring points after the equivalence point too.

For the recognition of the EPs found the set EP criterion is compared with the ERC (**E**quivalence point **R**ecognition **C**riterion) found. The ERC is the first derivative of the titration curve combined with a mathematical function which is more sensitive for flat jumps than for steeper ones. EPs whose ERC is smaller than the set EP criterion will not be recognized. The ERC for each found and recognized EP will be shown under **Results/Curve/EP Details**. If you subsequently adapt the EP criterion so that more or fewer EPs are recognized, you can trigger the **re-evaluation** under **Results** with [**Recalculate**].

Curve / EP details			
01 DET U Dynamic U titration			
Endpoint 1			
Volume	2.7098 mL	EP1	
Measured value	-19.7 mV	EM1	
ERC	67.5	EF1	
Time	41.7 s	ED1	
Temperature	25.0 °C	ET1	
Endpoint 2			
Volume	5.2237 mL	EP2	
Measured value	-207.9 mV	EM2	
ERC	15.4	EF2	
Time	83.1 s	ED2	
Temperature	25.0 °C	ET2	

For dynamic equivalence point titrations you can also show the ERC in addition to the titration curve. If the difference between the ERCs of the endpoints is large enough you will also be able to read off a sensible value for the EP criterion from the curve.



In the example shown an EP criterion of 20 would make sense if only the first equivalence point is to be recognized.

Evaluation and equivalence point criterion in the MET mode

The equivalence points (EPs) are localized by a procedure based on the Fortuin method which has been adapted by Metrohm for numerical methods. A search is made for the largest measured value alteration (Δ_n). The exact EP is determined by using an interpolation factor ρ ; this depends on the Δ -values before and after Δ_n :

$$V_{EP} = V_0 + \rho \Delta V$$

V_{EP} = EP volume, V_0 = total volume added before Δ_n , ΔV = volume increment, ρ = interpolation factor according to Fortuin

For the recognition of the EPs found the set EP criterion is compared with the ERC (**E**quivalence point **R**ecognition **C**riterion) found. The ERC is the sum of the measured value alterations before and after the jump:

$$|\Delta_{n-2}| + |\Delta_{n-1}| + |\Delta_n| + |\Delta_{n+1}| + |\Delta_{n+2}|$$

(In certain cases only three or only a single summand are taken into account.)

EPs whose ERC is smaller than the set EP criterion will not be recognized. The ERC for each found and recognized EP will be shown under **Results/Curve/EP Details**. If you subsequently adapt the EP criterion so that more or fewer EPs are recognized, you can trigger the **re-evaluation** under **Results** with **[Recalculate]**.

Curve / EP details			
01 MET U Monotonic U-Titration			
Endpoint 1			
Volume	2.7103 mL		EP1
Measured value	-13.3 mV		EM1
ERC	129.4 mV		EF1
Time	57.9 s		ED1
Temperature	25.0 °C		ET1
Endpoint 2			
Volume	5.2320 mL		EP2
Measured value	-208.4 mV		EM2
ERC	19.6 mV		EF2
Time	110.9 s		ED2
Temperature	25.0 °C		ET2

The parameters for **Control device**, **Sensor**, **Dosing device** and **Stirrer** are described in *Section 4.1.5*.

Titration sequence for DET and MET

Start of titration command	
(Switch on stirrer)	The stirrer is switched on after the start.
Measure initial measured value	The initial measured value is measured.
(Start conditions: start volume start meas. value start slope pause)	The start volume is added with the start conditions being processed in succession. No measuring points are entered in the list of measuring points. The pause interval is allowed to elapse.
Titration: add increments accept measured values	Volume increments are added during the titration and a measuring point is entered on the list of measuring points after each increment. Measured value acceptance is either drift-controlled (equilibrium titration) or a fixed waiting time is allowed to elapse. The first criterion to be fulfilled applies.
Stop conditions	The first criterion to be fulfilled applies for stopping the titration.
(Switch off stirrer)	The stirrer is switched off.
Fill dosing cylinder	After the end of the titration the dosing cylinder is refilled automatically.

Optional steps are shown in brackets.

4.1.2 Endpoint titrations (SET)

Start conditions

Under **Start conditions** the parameters for the start volume of titrant and for the measurement of the initial measured value are edited:

- **Pause 1** (d): Waiting time, e. g. for electrode equilibration, before a start volume is added.
- **Start volume** (d): Volume which is added before the start of the titration. Under **Dosing rate** (d) you can enter the rate at which the start volume is added.
- **Pause 2** (d): Waiting time which is allowed to elapse before the start of the titration after the start volume has been added.

Parameters for the **Initial measured value**:

- **Signal drift** (d): Drift, i.e. alteration in the measured value per minute, which has to be reached before the measured value will be accepted.
- **Waiting time min.** (d): The measured value is not accepted until the minimum waiting time has elapsed, even if the measured value drift has already been reached. The minimum waiting time is only important for drift-controlled measurements.
- **Waiting time max.** (d): If the signal drift is switched off or has not yet been reached then the measured value will be accepted after the maximum waiting time has elapsed.

Control parameters

Editing the **Control parameters** for endpoint 1 and endpoint 2:

- **EP1 at** (d): Measured value for the first endpoint.
- **Titration rate** (d): Three predefined sets of parameters can be selected for the titration rate (see Table on following page). If individual titration parameters need to be adapted you should select the setting **User** and edit the individual titration parameters under **User-defined Parameters**.

User-defined parameters

Editing the **User-defined Parameters**:

- **Dynamics** (d): The dynamics defines the measured value range (control range) before the preset endpoint. In the control range dosing is controlled by the **Minimum rate**. The closer the endpoint, the slower the dosing until the **Minimum rate** has been reached. The larger the control range, the slower the titration. Outside the control range dosing is carried out continuously at the **Maximum rate**.
- **Maximum rate** (d): Rate at which dosing is carried out outside the control range. The maximum dosing rate depends on the cylinder volume of the exchange or dosing unit used (see *Section 3.8.6*).
- **Minimum rate** (d): This parameter determines the dosing rate right at the start of the titration and in the **Dynamic** range at the end of the titration. It has a decisive influence on the titration rate and therefore on the accuracy. The smaller the selected minimum rate, the slower the titration.

Parameters for the predefined titration rates for SET

	Titration rate	slow	optimal	fast
SET	Control range (Dynamics)	5.000 pH 300.0 mV 40.0 μ A	2.000 pH 100.0 mV 10.0 μ A	0.500 pH 30.0 mV 5.0 μ A
	Max. rate	1.00 mL/min	10.00 mL/min	maximum
	Min. rate	5.00 μ L/min	25.00 μ L/min	50.00 μ L/min

Optimizing the control parameters

Reagent addition takes place in three phases during the titration:

- **Initial addition:** during this phase the dosing rate increases continuously. It starts with the **Minimum rate** and increases to the **Maximum rate**.
- **Continuous addition:** addition is carried out at the **Maximum rate** until the control range is reached.
- **Control range:** in this range addition is finely controlled. Shortly before the endpoint is reached addition is only carried out at the **Minimum rate**.

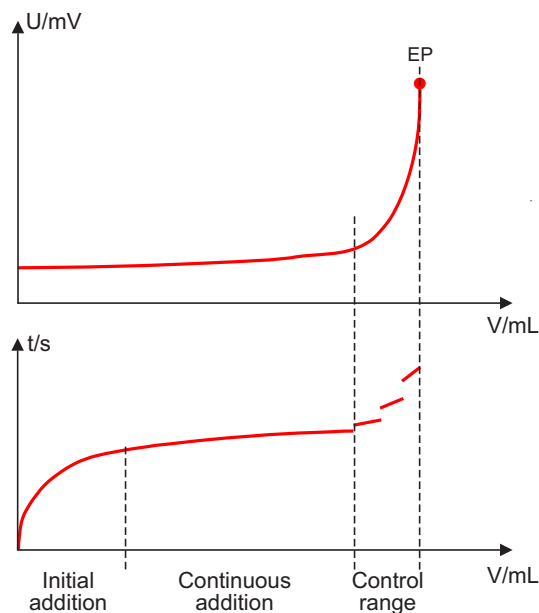


Fig. 4.8: Reagent addition during endpoint titrations with SET

Set a large **Control range** for steep curves and a small control range for flat ones. A good approximation for the start of the control range is given by the point where the tangents intersect:

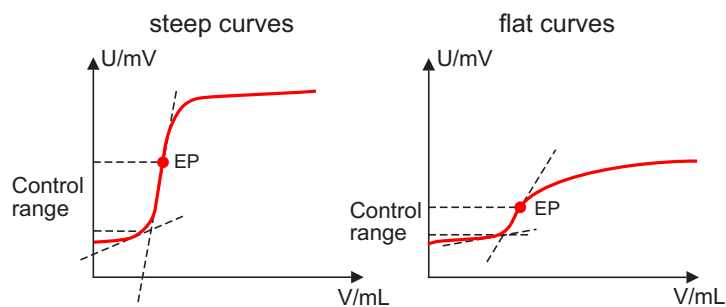


Fig. 4.9: Control range size

Stop criterion

Editing the parameters for the **Stop criterion**:

- **Stop criterion** (d): The titration stops when the endpoint has been reached and the stop criterion has been fulfilled. The titration can be stopped when a particular (volume) **drift** has been achieved or after a preset **time**. If no stop criterion has been selected the titration will not be stopped. The **Stop conditions** (see following page) will always stop the titration even if the stop criterion has not been fulfilled.
- **Stop drift** (d): If the endpoint and the stop drift have been reached the titration will be stopped.
- **Delay time** (d): After the endpoint has been reached the preset time will be allowed to elapse after the last addition before the titration is stopped.

In older instructions the Delay time was usually defined as the **Stop criterion**. The stop criterion **time** means that the endpoint must be exceeded for a certain time: the Delay time. The same Delay time with different very small volume increments (depending on the volume of the exchange or dosing unit, see below) means different switch-off points. In contrast, if **drift** is used as the stop criterion then the switch-off point will always have the same curve slope dV/dt .

You can use the switch-off time in the following way to calculate the maximum stop drift to be used: the size of the last increment to be added depends on the volume of the attached exchange unit. With a 20 mL exchange unit (10'000 pulses per cylinder volume) – number of impulses depends on the dosing device – the smallest possible increment is $2 \mu\text{L}$. With a delay time of 5 s this means that the last $2 \mu\text{L}$ of reagent to be added must be sufficient for 5 s or longer. This results in a drift of $\leq 2 \mu\text{L}/5 \text{ s} = 24 \mu\text{L}/\text{min}$. The drift can be smaller than $24 \mu\text{L}/\text{min}$ as we do not know whether the last increment would also have been sufficient for 10 s. This means that if you have previously worked with a 20 mL exchange unit (10'000 pulses per cylinder volume) and 5 s switch-off delay then you should set a value of $\leq 24 \mu\text{L}/\text{min}$ as the stop drift.

End point 2

The control parameters for Endpoint 2 are the same as for Endpoint 1.

Titration parameters

The parameters for the titration sequence are edited under **Titration parameters**:

- **Titration direction** (d): The titration direction is normally determined automatically from the initial measured value and the set endpoint. It is recommended that, whenever possible, a positive or negative alteration of the measured value is entered. If two endpoints have been set then the titration direction will be defined automatically. In this case the setting will be ignored.
- **Extraction time** (d): The titration takes place during this time. The titration will not be stopped until the extraction time has elapsed (even if the EP has already been reached). The entry of an extraction time may be advisable, e. g. for the titration of sparingly soluble samples.
- **Temperature** (d): Manually entered titration temperature. If a temperature sensor is connected and temperature measurement is set to **automatic** or **continuous** under **Sensor** (see *Section 4.1.5*) then the temperature will be measured continuously. The value is used for temperature compensation in pH measurements.
- **Time interval MP** (d): Time interval for entering a measuring point in the list of measuring points.

Stop conditions

The conditions for terminating the titration are defined under **Stop conditions** if this does not occur automatically because either the set endpoint has not been reached or the stop criterion has not been fulfilled:

- **Stop volume** (d): Stops when the preset volume has been added since the start of the titration. You should adapt the stop volume to suit the size of your titration vessel in order to prevent it from overflowing.
- **Stop time** (d): Stops when the preset time has elapsed after the start conditions have been fulfilled.

If several stop conditions have been set then the first criterion to be fulfilled will stop the titration.

- **Filling rate** (d): Rate at which the dosing cylinder is refilled after the titration. The maximum filling rate depends on the cylinder volume of the exchange or dosing unit used (see *Section 3.8.6*).

Conditioning

Under **Conditioning** (d) the conditions for pre- and reconditioning are defined. With conditioning switched on, the first time that the method is started only the command to start conditioning will be executed. None of the other commands will be processed yet. The solution in the titration cell is titrated to the endpoint with the given control parameters and is then kept there continuously. The method sequence itself only starts when **[Start]** is pressed again.

- **Start drift** (d): As soon as this volume drift is undercut "Conditioning OK" appears and the titration method can be started.
- **Drift correction** (d): The EP-volume can be drift-corrected. With **auto** the volume drift value at the start of the titration will be taken over automatically, multiplied by the drift correction time and subtracted from the EP-volume. The drift correction time is the time in-

interval between the end of conditioning and the end of the determination. If the drift is known for a longer period of time then this can be calculated for the EP-volume by **manual** drift correction. The result always indicates whether it has been drift-corrected or not.

- **Drift value** (d): Volume drift for manual drift correction
- **Measured value display**: The volume drift can be shown continuously during conditioning.

Cond.
options

Editing the **conditioning options**:

- **Cond. stop volume**: If the entered volume has been added before conditioning has been completed then the process will be stopped. If conditioning is continued by pressing **[Start]** again then the titrant volume that has already been added will not be taken into account; addition starts again from zero. The stop volume should be adapted to the size of the titration cell in order to prevent any overflow.
- **Cond. stop time**: If conditioning takes longer than the time entered here then the process will be stopped.
- **Start reconditioning at end of method**: If this option is switched on then reconditioning will only start when all method commands have been processed. Otherwise reconditioning would start immediately after the titration command. This function must be activated if other commands follow the SET command that must not be allowed to take place at the same time as conditioning. Example: emptying the titration cell and then adding new solution.

The parameters for **Control device**, **Sensor**, **Dosing device** and **Stirrer** are described in *Section 4.1.5*.

Titration sequence for SET

1st start of titration command	Checks whether work is to be carried out with or without conditioning.
(Switch on stirrer)	The stirrer is switched on after the start.
Preconditioning (if activated)	The titration cell solution is titrated to the endpoint and kept there continuously.
2nd start of titration command	The method sequence itself starts.
Measure initial measured value	The initial measured value is measured.
(Start conditions: Pause 1 Start volume Pause 2)	Pause interval 1 is allowed to elapse. The start volume is added. No measuring points are entered in the list of measuring points. Pause interval 2 is allowed to elapse.
(Extraction time) Titration with test up to stop when stop criterion or the stop condition is reached	Titration is carried out to the first and then to the second endpoint. If the extraction time has not elapsed when the (first) endpoint has been reached then it will be allowed to elapse and the titration (to the first endpoint) will only be concluded when the extraction time has elapsed.
(Switch off stirrer)	The stirrer is switched off if there is no reconditioning.
Fill dosing cylinder	After the end of the titration the dosing cylinder is refilled automatically.
Reconditioning	The titration cell solution is kept continuously at the endpoint.

Optional steps are shown in brackets.

4.1.3 Karl Fischer titrations (KFT)

Start conditions

Under **Start conditions** the parameters for the addition of the start volume of titrant and for measuring the initial measured value are edited. These conditions must be fulfilled before a titration can be started.

- **Pause 1** (d): Waiting time, e. g. for electrode equilibration, before the start volume is added.
- **Start volume** (d): Volume which is added before the start of the titration. Under **Dosing rate** (d) the rate at which the start volume is added is entered.
- **Pause 2** (d): Waiting time which is allowed to elapse between adding the start volume and starting the titration.

Parameters for the **Initial measured value**:

- **Signal drift** (d): Drift, i.e. alteration of the measured value per minute, which has to be reached before the measured value will be accepted.
- **Waiting time min.** (d): The measured value is not accepted until the minimum waiting time has elapsed, even if the measured value drift has already been reached. The minimum waiting time is only important for drift-controlled measurements.
- **Waiting time max.** (d): If the signal drift is switched off or has not yet been reached then the measured value will be accepted after the maximum waiting time.

Control parameters

Editing the **Control parameters** for the endpoint:

- **Endpoint at** (d): Measured value for the end-point.
- **Titration rate** (d): Three predefined sets of parameters can be selected for the titration rate (see Table on following page). If individual titration parameters need to be adapted then select the setting **User** and edit the individual titration parameters under **User-defined parameters**.

User-defined parameters

Editing the **User-defined parameters**:

- **Dynamics** (d): The dynamics defines the measured value range (control range) before the given endpoint. In the control range dosing is controlled by the **minimum increment**. The closer the endpoint, the slower the dosing until the **minimum increment** has been reached. The larger the control range, the slower the titration. Outside the control range dosing takes place at the **maximum rate**.
- **Maximum rate** (d): Rate at which dosing takes place outside the control range. The maximum rate depends on the cylinder volume of the exchange or dosing unit used (see Section 3.8.6).
- **Minimum increment** (d): This parameter determines the volume steps at which addition takes place right at the start of the titration and in the **control range** at the end of the titration. It has a decisive influence on the titration rate and therefore on the accuracy. The smaller the selected minimum increment, the slower the titration.

Parameters for the predefined titration rates for KFT

	Titration rate	slow	optimal	fast
KFT	Control range (Dynamics)	300.0 mV 40.0 μ A	100.0 mV 10.0 μ A	30.0 mV 5.00 μ A
	Max. rate	1.00 mL/min	maximum	maximum
	Min. increment	minimum (= cylinder volume/10000)	minimum (= cylinder volume/10000)	5.00 μ L

Stop criterion

Editing the parameters for the **Stop criterion**:

- **Stop criterion** (d): When the endpoint has been reached and the stop criterion has been fulfilled the titration is stopped. The titration can be stopped when a certain (volume) **drift** has been reached or after a certain **time**. If no stop criterion has been selected then the titration will not be stopped. The **Stop conditions** (see following page) will always ensure a stop, even if the stop criterion has not been reached.
- **Stop drift** (d): When the endpoint and the stop drift have been reached the titration is stopped.
- **Delay time** (d): When the endpoint has been reached the given time will be allowed to elapse after the last addition and the titration will then be stopped.
- **Relative stop drift** (d): When the endpoint and the sum of the drift at the start of the titration and the rel. stop drift have been reached then the titration will be stopped.

You can use the Delay time to calculate the maximum stop drift to be used in the following way: the size of the last added increment depends on the volume of the attached exchange unit. With a 20 mL exchange unit (10'000 pulses per cylinder volume; for KFT command is independent of the dosing drive) the smallest possible increment is 2 μ L. With a Delay time of 5 s the last 2 μ L of reagent must therefore suffice for 5 s or longer. This gives a drift of $\leq 2 \mu\text{L}/5 \text{ s} = 24 \mu\text{L}/\text{min}$. (The drift may be smaller than 24 $\mu\text{L}/\text{min}$ as we do not know whether the last increment would also have been sufficient for 10 s.) This means that if you use a 20 mL exchange unit (10'000 pulses per cylinder volume; independent of the dosing drive) and 5 s switch-off delay then you should set a value of $\leq 24 \mu\text{L}/\text{min}$ as the stop drift.

Titration parameters

Under **Titration parameters** the parameters for the titration sequence are edited:

- **Titration direction** (d): A direction is normally given as standard. With **auto** the titration direction is determined from the initial measured value and the set endpoint.
- **Extraction time** (d): The titration continues during this time. The titration is not stopped until the extraction time has elapsed (even

when the EP has already been reached). The entry of an extraction time is advisable for samples which only release their water slowly.

- **Temperature** (d): Manually entered titration temperature. If a temperature sensor is connected and the temperature measurement is set to **automatic** or **continuous** under **Sensor** (see *Section 4.1.5*) then the temperature will be measured continuously.
- **Time interval MP** (d): Time interval for entering a measuring point in the list of measuring points.

Stop conditions

Under **Stop conditions** the conditions for stopping the titration are defined should this not take place "normally". This could happen when the set endpoint is not reached or if the stop criterion is not fulfilled.

- **Stop volume** (d): Stops when the entered volume has been added since the start of the titration. Adapt the size of the stop volume to the size of your titration cell to prevent an overflow.
- **Stop time** (d): Stops when the entered time has elapsed after the start conditions have been fulfilled.

If several stop conditions have been set then the first of them to occur will stop the titration.

- **Filling rate** (d): Rate at which the dosing cylinder is refilled after the titration. The maximum filling rate depends on the cylinder volume of the exchange or dosing unit used (see *Section 3.8.6*).

Conditioning

Under **Conditioning** (d) the conditions for pre-and reconditioning are defined. With conditioning switched on, the first time that the method is started only the command to start conditioning will be executed. None of the other commands will be processed yet. The solution in the titration cell is titrated to the endpoint with the given control parameters and is then kept there continuously. The method sequence itself only starts when **[Start]** is pressed again.

- **Start drift** (d): As soon as this volume drift is undercut "Conditioning OK" appears and the titration method can be started.
- **Drift correction** (d): The EP-volume can be drift-corrected. With **auto** the volume drift value at the start of the titration will be taken over automatically, multiplied by the drift correction time and subtracted from the EP-volume. The drift correction time is the time interval between the end of conditioning and the end of the determination. If the drift is known for a longer period of time then this can be calculated for the EP-volume by **manual** drift correction. The result always indicates whether it has been drift-corrected or not.
- **Drift value** (d): Volume drift for manual drift correction
- **Measured value display**: The volume drift can be shown continuously during conditioning.

Cond. options

Editing the **conditioning options**:

- **Cond. stop volume**: If the entered volume has been added before conditioning has been completed then the process will be stopped. If conditioning is continued by pressing **[Start]** again then the titrant volume that has already been added will not be taken into account; addition starts again from zero. The stop volume should be

adapted to the size of the titration cell in order to prevent any overflow.

- **Cond. stop time:** If conditioning takes longer than the time entered here then the process will be stopped.
- **Start reconditioning only at end of method:** If this option is switched on then reconditioning will only start when all method commands have been processed. Otherwise reconditioning would start immediately after the titration command. This function must be activated if other commands follow the KFT command that must not be allowed to take place at the same time as conditioning. Example: emptying the titration cell and then adding new solution.

The parameters for **Control device**, **Sensor**, **Dosing device** and **Stirrer** are described in *Section 4.1.5*.

Titration sequence for KFT

1st start of titration command	Checks whether work is to be carried out with or without conditioning.
(Switch on stirrer)	The stirrer is switched on after the start.
Preconditioning (if activated)	The titration cell solution is titrated to the endpoint and kept there continuously.
2nd start of titration command	The method sequence itself starts.
Measure initial measured value	The initial measured value is measured.
(Start conditions: Pause 1 Start volume Pause 2)	Pause interval 1 is allowed to elapse. The start volume is added. No measuring points are entered in the list of measuring points. Pause interval 2 is allowed to elapse.
(Extraction time) Titration with test up to stop when stop criterion or the stop condition is reached	Titration is carried out. If the extraction time has not elapsed when the endpoint has been reached then it will be allowed to elapse and the titration will only be concluded when the extraction time has elapsed.
(Switch off stirrer)	The stirrer is switched off if there is no reconditioning.
Fill dosing cylinder	After the end of the titration the dosing cylinder is refilled automatically.
Post-conditioning	The titration cell solution is kept continuously at the endpoint.

Optional steps are shown in brackets.

4.1.4 STAT titrations (STAT)

Start conditions

Under **Start conditions** the parameters for the start volume of titrant and for the measurement of the initial measured value are edited:

- **Pause 1:** Waiting time, e. g. for electrode equilibration, before a start volume is added.
- **Start volume:** Volume which is added before the start of the titration. Under **Dosing rate** you can enter the rate at which the start volume is added.
- **Pause 2:** Waiting time which is allowed to elapse before the start of the titration after the start volume has been added.

Parameters for the **Initial measured value**:

- **Signal drift:** Drift, i.e. alteration in the measured value per minute, which has to be reached before the measured value will be accepted.
- **Waiting time min.:** The measured value is not accepted until the minimum waiting time has elapsed, even if the measured value drift has already been reached. The minimum waiting time is only important for drift-controlled measurements.
- **Waiting time max.:** If the signal drift is switched off or has not yet been reached then the measured value will be accepted after the maximum waiting time has elapsed.

Control parameters

Editing the **Control parameters** for the control point:

- **Control point at:** Measured value for the control point.
- **Titration rate:** Three predefined sets of parameters can be selected for the titration rate (see Table on following page). If individual titration parameters need to be adapted you should select the setting **User** and edit the individual titration parameters under **User-defined Parameters**.

User-defined parameters

Editing the **User-defined Parameters**:

- **Dynamics:** The dynamics defines the measured value range (control range) before the preset control point. In the control range dosing is controlled by the **Minimum rate**. The closer the control point, the slower the dosing until the **Minimum rate** has been reached. The larger the control range, the slower the titration. Outside the control range dosing is carried out continuously at the **Maximum rate**.
- **Maximum rate:** Rate at which dosing is carried out outside the control range. The maximum dosing rate depends on the cylinder volume of the exchange or dosing unit used (see *Section 3.8.6*).

Rule of thumb for the maximum rate:

$$\text{Max. rate in mL/min} = 0.005 \cdot \text{expected rate of reaction in } \mu\text{L/min}$$

- **Minimum rate:** This parameter determines the minimum dosing rate right at the start of the titration and in the **Dynamic** range at the end of the titration. It has a decisive influence on the behavior at the control point. The minimum rate also has a decisive influence on how exactly the control point can be kept constant. The smaller the

selected minimum rate, the longer it takes until the control point is reached for the first time.

The following rule of thumb should be considered in order to obtain as constant a dosing at the control point as possible:

$$\text{Min. rate in } \mu\text{L/min} = \frac{\text{Expected rate of reaction in } \mu\text{L/min}}{10}$$

Parameters for the predefined titration rates for STAT

	Rate of reaction	50 $\mu\text{L/min}$	100 $\mu\text{L/min}$	500 $\mu\text{L/min}$
STAT	Control range (Dynamics)	1.000 pH 60.0 mV	1.000 pH 60.0 mV	1.000 pH 60.0 mV
	Max. rate	0.25 mL/min	0.75 mL/min	2.00 mL/min
	Min. rate	5.00 $\mu\text{L/min}$	10.00 $\mu\text{L/min}$	40.00 $\mu\text{L/min}$

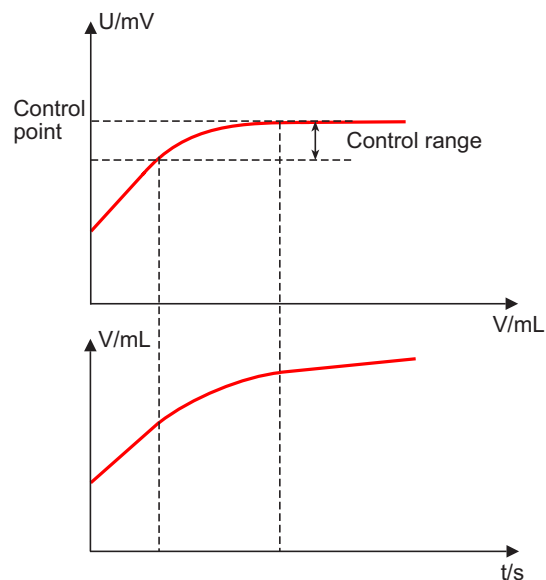


Fig. 4.10: Reagent addition and control range for STAT

Dosing outside the control range:

Outside the control range the dosing rate is mainly characterized by the **maximum rate**. The parameters **maximum rate** and **dynamics** should be optimized together in such a way that the titration does not overshoot too much when reaching the control point. The control range should be set so that the measured value remains within this range while it is kept constant. A slightly larger control range should be defined for slow reactions (e. g. pH = 3, U = 180 mV). A SET pretitration is frequently used to reach the control point before the substrate is added. This means that the STAT titration can be started with a small variation from the control point.

Dosing within the control range:

Within the control range the dosing rate is mainly characterized by the **minimum rate**.

Titration parameters

The parameters for the titration sequence are edited under **Titration parameters**:

- **Titration direction:** The titration direction is normally determined automatically from the initial measured value and the set control point. It is recommended that, whenever possible, a positive or negative alteration of the measured value is entered.
- **Temperature:** Manually entered titration temperature. If a temperature sensor is connected and temperature measurement is set to **automatic** or **continuous** under **Sensor** (see *Section 4.1.5*) then the temperature will be measured continuously. The value is used for temperature compensation in pH measurements.
- **Time interval MP:** Time interval for entering a measuring point in the list of measuring points.
- **Start time:** The measured values are not entered in the list of measuring points until this time has elapsed since the start of the titration.
- **Start measured value:** The measured values are not entered in the list of measuring points until this value has been reached.
- **Start rate:** The measured values are not entered in the list of measuring points until the dosing rate has fallen below this value. This parameter is checked 10 s after the start at the earliest.

If several start parameters have been defined, all of them must be fulfilled for a measured value to be entered in the list of measuring points.

Stop conditions

The conditions for terminating the titration are defined under **Stop conditions**:

- **Stop volume:** Stops when the preset volume has been added since the start of the titration.
- **Stop time:** Stops when the preset time has elapsed after the start conditions have been fulfilled.
- **Since:** Specifies the beginning of the stop time.
Start: The stop time starts after the start conditions have been fulfilled.
Control reached: The stop time starts as soon as the control point has been reached for the first time.
Last dosing: The stop time starts after the last increment has been dosed, i.e. the stop time is reset to zero again after each dosing step.
- **Stop rate:** Stops when the current titration rate is lower than the rate defined here.

If several stop conditions have been set then the first criterion to be fulfilled will stop the titration.

- **Filling rate:** Rate at which the dosing cylinder is refilled after the titration. The maximum filling rate depends on the cylinder volume of the exchange or dosing unit used (see *Section 3.8.6*).

Monitoring

Under **Monitoring** the parameters for monitoring the **measured value**, the **dosing rate** (an average rate) as well as the **temperature** are defined. Remote signals or RS commands can be assigned to the monitored quantities. This can be used, for example, to switch a thermostat on/off if necessary. Monitoring is not used for parameterization of the control behavior.

The following parameters are identical for all monitored quantities.

- **Monitoring:** The monitoring of the corresponding parameter is switched on or off. The monitoring of the dosing rate starts 10 s after the start of the titration at the earliest.
- **Lower limit:** When the monitored quantity falls below this value, a certain action (see below) is triggered.
- **Lower hysteresis:** The lower hysteresis represents a tolerance range for the lower limit (see *Fig. 4.13*). With the **action "Wait"** dosing does not continue until the monitored quantity has exceeded the lower limit plus this value. Only positive values are allowed.
- **Upper limit:** A certain action (see below) is triggered if this value is exceeded.
- **Upper hysteresis:** The upper hysteresis represents a tolerance range for the upper limit (see *Fig. 4.13*). With the **action "Wait"** dosing does not continue until the monitored quantity has fallen below the upper limit minus this value. Only positive values are allowed.
- **Action:** Definition of the action to be taken when the limits of the monitored quantity are infringed. With the actions **Hold** and **Wait** the other quantities continue to be monitored in the background.

No action will be taken with **None**.

The method is stopped immediately with **Exit method**.

The current command (STAT, DOS) is quit and the following command in the method is started with **Skip command**.

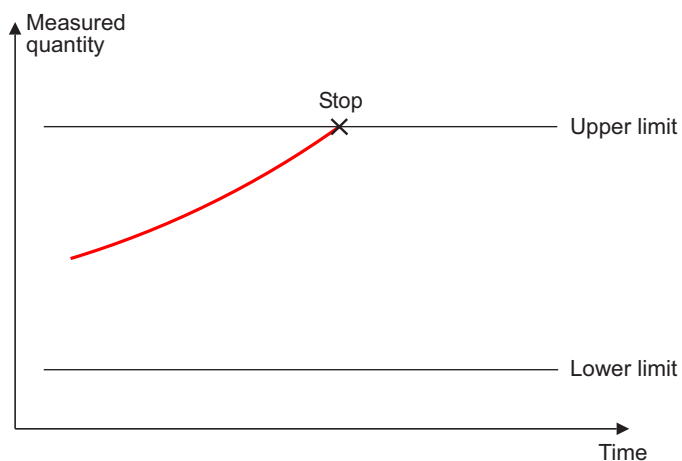


Fig. 4.11: Action "Exit method" or "Skip command"

When selecting **Hold**, the addition of the reagent is interrupted until the method sequence is continued manually with **[Continue]**. If the monitored quantity is still outside the limits (including hysteresis), it is not possible to continue the method sequence.

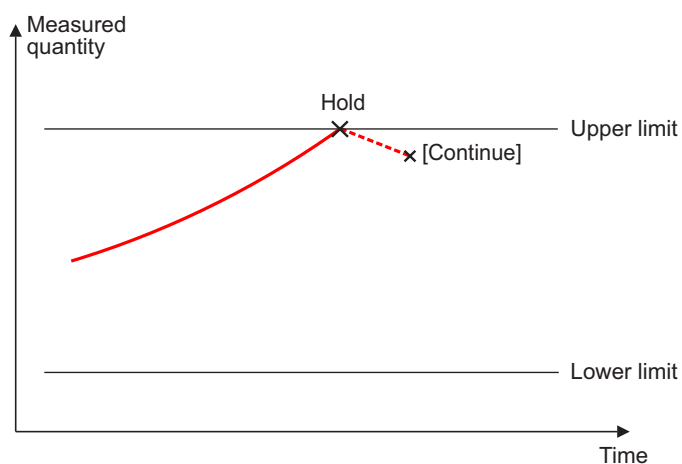


Fig. 4.12: Action "Hold"

When selecting **Wait**, the addition of the reagent is interrupted until the monitored quantity is within the limits (including hysteresis) again. The dosing is continued automatically.

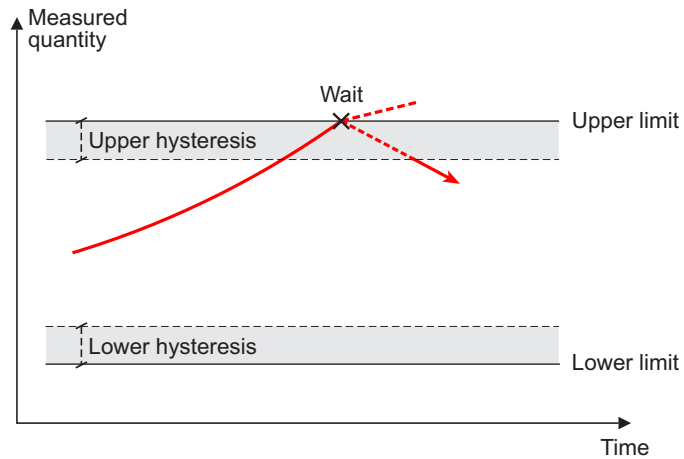


Fig. 4.13: Action "Wait"



Note!

If the lower limit is infringed while monitoring the dosing rate, the actions **Hold** and **Wait** do not make sense because the average dosing rate becomes smaller and smaller during the waiting time. The valid range can never be reached again.

Communication

Under **Communication** a monitored quantity can be assigned to a remote output signal or to an RS-232 command. Open the editing dialog with **[New]**:

- **Assignment:** Select the monitored quantity which should be assigned to a remote interface or a serial interface. If several quantities are monitored, with **any** the defined output signal or the data string is sent as soon as a limit of one of the monitored quantities is infringed.
- **Infringed limit:** Specify the limit whose infringement causes the signal or data string defined below to be sent. Select **any** if the signal or data string should be sent if either of the two limits has been infringed. Select **back in range** if the signal or data string should be sent as soon as the monitored quantity is within the limits (including hysteresis) again.
- **Interface:** Select the remote box or the serial interface via which the signal or data string should be sent.
- **Output signal:** Select the signal from the templates (defined under **System/Templates/Output lines**) or enter the desired binary pattern (please see online help and CTRL command). A set remote line is not reset automatically at the end of the determination.
- **Data string:** Enter the desired data string. All characters according to ASCII code can be used. Please consult the online help for how to enter the data string.



Note!

The signal or the data string is sent for all actions defined under **[Monitoring]**.

The parameters for **Control device**, **Sensor**, **Dosing device** and **Stirrer** are described in the following Section.

Titration sequence for STAT

Start of titration command	
(Switch on stirrer)	The stirrer is switched on after the start.
Measure initial measured value	The initial measured value is measured.
(Start conditions: Pause 1 Start volume Pause 2)	Pause interval 1 is allowed to elapse. The start volume is added. No measuring points are entered in the list of measuring points. Pause interval 2 is allowed to elapse.
Titration	Titration to the control point is carried out. During this time controlling is active as well as monitoring. Measured values are not entered in the list of measuring points until the titration parameters (Start time, Start measured value, Start rate) are fulfilled.
Stop conditions	The first criterion to be fulfilled applies for stopping the titration.
(Switch off stirrer)	The stirrer is switched off.
Fill dosing cylinder	After the end of the titration the dosing cylinder is refilled automatically.

Optional steps are shown in brackets.

4.1.5 Control device, sensor, dosing device and stirrer

Control device

Under **Control device** you can select the Titrando or the Robotic Titrator with which the titration (or measurement or calibration) is to be carried out. This button will only appear when several control devices that are able to execute the corresponding command have been configured under **System/Device manager** (see *Section 3.10*). The instrument names are always shown in the selection list.

Sensor

The parameters for the electrode connection are edited under **Sensor**:

- **Measuring input** (d): Selects the measuring input to which the sensor is connected. The choice is not dependent on whether the Titrando has one or two measuring inputs.
- **Sensor** (d): Selects the sensor from the sensor list defined under **System/Sensors**. The selection depends on the quantity to be measured (see **online help**). You can also enter a sensor name which is not contained in the sensor list. However, the sensor must be present in the sensor list when the determination is carried out.
- **I(pol)** (d): The polarization current is the current applied to the polarizable electrode during a voltametric measurement. This parameter is only available for I(pol) titrations/measurements.
- **U(pol)** (d): The polarization voltage is the voltage applied to the polarizable electrode during an amperometric measurement. This parameter is only available for U(pol) titrations/measurements.
- **Electrode test** (d): The electrode test for polarizable electrodes is carried out during the transition from an inactive condition to a measuring condition. A check is made that the electrode is properly connected and that no short-circuit is present.
- **Temperature measurement** (d):

The temperature is normally measured **automatically** if a temperature sensor is connected. Otherwise the temperature entered manually under **Temperature** (Titration/Measuring/Dosing parameters) will be used.

With **continuous** you can ensure that a temperature sensor must be connected.

With **off** the temperature entered manually under **Temperature** will always be used. In case of electrode calibration and the electrode test, the temperature is requested after the start, except the determination is carried out with a Sample Processor.

Dosing device

The parameters for the dosing device are edited under **Dosing device**:

- **Dosing device** (d): Selects the dosing device to be used for the titration. All the dosing device connections (MSB) are always shown.
- **Titrant** (d): Titrant to be used for the titration (or dosing). The titrant can be selected from the list of titrants which have been defined under **System/Titrants**. If intelligent exchange or dosing units are used then a check will be made in the method sequence that the correct titrant is present in the connected dosing device and whether the type of dosing device is correct. With non-intelligent exchange or dosing units the cylinder volume is checked.

At the start of the titration the validity of the titer and the expiry date of the selected titrant will be checked as well as the GLP test interval for the exchange or dosing unit. The titer (Variable TITER) and the concentration (Variable CONC) are also available for calculation (CALC command, see *Section 4.5.1*).

Tandem dosing

STAT, ADD, DOS only: A second dosing device can be defined under **Tandem dosing** in order to enable continuous dosing. Dosing is carried out with a combination of two dosing devices so that the second dosing device is dosing while the first one is being filled and vice versa.

- **Dosing device:** Select the second dosing device.
- **Titration:** See above. The concentration, the validity of the titer and the working life are ignored in contrast to the titration of the first dosing device.
- **Filling rate:** Rate at which the dosing cylinder of the second dosing device is filled. The maximum filling rate depends on the cylinder volume of the exchange or dosing unit used (see *Section 3.8.6*).

However, in order to ensure continuous dosing, the following points must be taken into account:

- Use the highest possible filling rate in order to keep the filling times as short as possible. Please note the viscosity and density of the liquid.
- When you use two dosing devices with different cylinder volumes the filling rate of the larger cylinder must be at the minimum:

$$\text{Filling rate 2} \geq \text{Filling rate 1} \cdot \frac{V_{\text{Dos.cyl.2}}}{V_{\text{Dos.cyl.1}}}$$

Example:

Dosing device 1: Volume = 20 mL, Filling rate = 50 mL/min

Dosing device 2: Volume = 50 mL

$$\text{Filling rate 2} \geq 50 \text{ mL/min} \cdot 50 \text{ mL}/20 \text{ mL} \geq 125 \text{ mL/min}$$

- The dosing rate must not exceed 75 % of the filling rate of the smaller cylinder. This corresponds to the following values (at the maximum filling rate):

Cylinder volume	Max. dosing rate		Max. flow rate	
	Exchange unit	Dosing unit	Exchange unit	Dosing unit
1 mL	2.25 mL/min	---	approx. 130 mL/h	---
2 mL	---	5.00 mL/min	---	approx. 300 mL/h
5 mL	11.25 mL/min	12.50 mL/min	approx. 670 mL/h	approx. 750 mL/h
10 mL	22.50 mL/min	25.00 mL/min	approx. 1.3 L/h	approx. 1.5 L/h
20 mL	45.00 mL/min	50.00 mL/min	approx. 2.7 L/h	approx. 3.0 L/h
50 mL	112.50 mL/min	124.50 mL/min	approx. 6.7 L/h	approx. 7.5 L/h

The dosing rate corresponds to the flow rate for continuous dosing.

Stirrer

The parameters for the stirrer are edited under **Stirrer**:

- **Stirrer** (d): Selects the stirrer to be used in the titration (or measurement, calibration, dosing). All the stirrer connections (MSB) will always be shown.
- **Stirring rate** (d): You can check the optimal stirring rate manually (see Section 3.24.3). The stirring direction changes as the sign changes. The default setting **8** corresponds to 1000 rpm (see Fig. 4.14).
- **Switch off automatically** (d): This function is used to switch off the stirrer automatically at the end of the titration (or measurement, calibration, dosing).

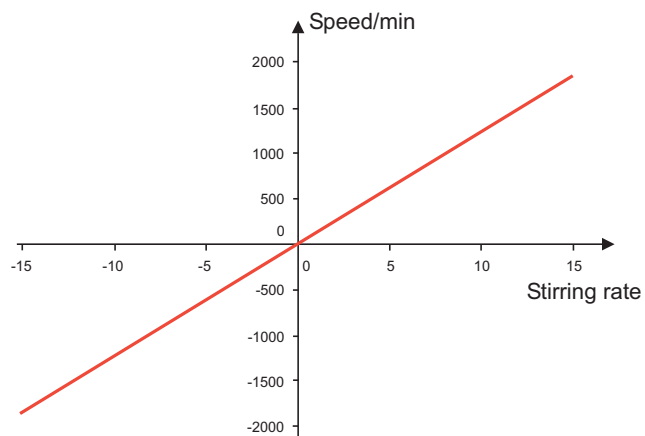


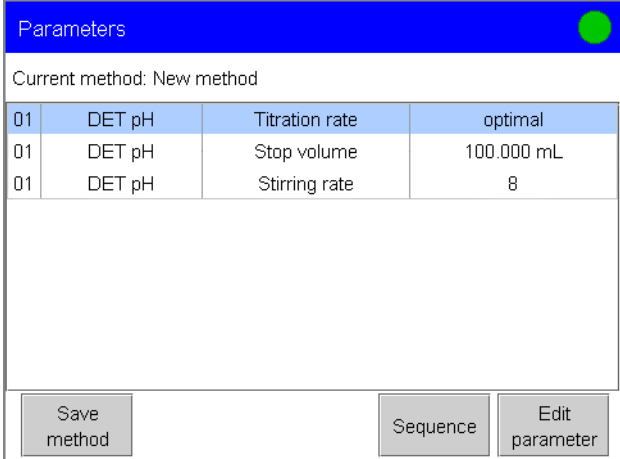
Fig. 4.14: Setting the stirring rate and speed

4.1.6 Direct parameters

Direct parameters can be defined for all titration commands; these are then shown in a table when the parameter dialog is opened and can be edited directly (see *Section 3.16.5*). Direct access ("**Quick Access**") to the edit dialog for selected method parameters simplifies the editing of parameters which need frequent alteration.

Direct parameters

You can define the parameters to be shown in the list of direct parameters under **Direct parameters**. For titrations these are all the parameters except those used for setting windows.



Parameters

Current method: New method

01	DET pH	Titration rate	optimal
01	DET pH	Stop volume	100.000 mL
01	DET pH	Stirring rate	8

Save method Sequence Edit parameter

4.2 Measurements (MEAS)

The following measuring modes can be selected:

- pH (potentiometric pH measurement)
- U (potentiometric voltage measurement)
- T (temperature measurement)
- I_{pol} (voltametric measurement with adjustable polarization current)
- U_{pol} (amperometric measurement with adjustable polarization voltage)
- Conc (concentration measurement)
- Cond (conductivity measurement, see Section 4.3).

Measuring parameters

The parameters for the measurement sequence are edited under **Measuring parameters**.

- **Signal drift (d)**: Drift, i.e. the alteration in the measured value per minute that has to be reached for measured value acceptance. **off** means that the measured value acceptance takes place when the maximum waiting time has elapsed. This may be advisable if the electrode has a very slow response.



Note!

A **constant measured value** is often only achieved after a certain time, as mixing and possibly the reaction itself require a certain time. The response time of an electrode can also increase with time, i.e. reaching a constant measured value takes longer and longer. In such a case **drift-controlled measured value acceptance** is particularly advisable, as the measured values are only accepted when equilibrium has almost been achieved.

- **Waiting time min. (d)**: The measured value is not accepted until the minimum waiting time has elapsed, even if the measured value drift has already been reached. The minimum waiting time is only important for drift-controlled measurements.
- **Waiting time max. (d)**: If the signal drift is switched off or has not yet been reached then the measured value will be accepted after the maximum waiting time has elapsed. If the waiting time has not been newly entered then a waiting time that is suitable for the drift will be calculated automatically according to the following equation:

$$\text{Waiting time} = 150 / \sqrt{\text{Drift} + 0.01} + 5$$

- **Stop measured value (d)**: Stops when the preset measured value has been reached since the start of the measurement.
- **Temperature (d)**: Manually entered measuring temperature. If a temperature sensor is connected and temperature measurement is set to **automatic** or **continuous** under **Sensor** (see Section 4.1.5) then the temperature will be measured continuously. The value is used for temperature compensation in pH measurements.
- **Time interval MP (d)**: Time interval for entering a measuring point in the list of measuring points. This list can contain max. 1000 measuring points.

**Note!**

The algorithm is only valid for direct measurements (MEAS Conc) if the following conditions are fulfilled:

- The **sample preparation** must be **identical** for the standards and the sample i.e. if aqueous standards have been used for the calibration of the sensor the sample has to be prepared in aqueous agent as well.
- The ratio **sample volume / volume auxiliary solution** must be identical with the ratio **standard volume / volume auxiliary solution** when calibrating the sensor.

Standard addition

This button is only available with the MEAS Conc command.

The parameters for concentration measurements by standard addition are edited under **Standard addition**.

- **Addition:** Select **off** if you wish to carry out a concentration measurement without standard addition i.e. as direct measurement.

The addition of the standard solution is done automatically with the setting **auto**. The individual addition increments are calculated and added in such a way that the constant potential difference **Delta U** defined under **[Dosing device]** is always achieved.

When selecting **auto dos** the addition of the standard solution is also done automatically but you can define the individual addition increments.

The standard solution is added manually with the setting **manual**. The volume of the increments is defined under **[Addition increments]**.

- **Conc. standard:** Input of the concentration of the standard solution and selection or input of the unit. If you have selected "**from list**" as concentration, you have to select the standard from the list of titrants under **[Dosing device]**.
- **No. of addition:** Number of standard additions. The evaluation becomes more accurate the more addition steps you carry out. At least four additions should be carried out.
- **Stop volume:** The sum of the addition increments must not exceed the stop volume defined here. Otherwise a corresponding error message will be displayed.
- **V aux. solution:** This is the volume of the buffer solution, etc. that needs to be added to the sample before the measurement can be started.

Stirrer control

Under **Stirrer control** you can edit the parameters for controlling the stirrer during the standard addition. Take care that you have selected a stirrer under **Edit command/Stirrer**.

- **Stir solution during measurement** (d): Automatically switches the stirrer on/off at the start and the end of the measurement.
- **Stir before meas.** (d): If stirring is switched off during the measurement, the solution can be stirred before the measurement. Enter the corresponding time here.

- **Pause before meas.** (d): If stirring is carried out before the measurement, a pause interval can be entered here. No stirring or measuring occurs during this time.

Dosing device

The parameters for the dosing device are defined under **Dosing device**.

- **Dosing device:** Selects the dosing device to be used for the standard addition. All the dosing device connections (MSB) are always shown.
- **Standard:** Standard to be used for the dosing. The standard can be selected from the list of titrants which have been defined under **System/Titrants**. In order to cope with the special situation of the standard addition the titrants are called standards here. If intelligent exchange or dosing units are used then a check will be made in the method sequence that the correct standard is present on the connected dosing device and whether the type of dosing device is correct. With non-intelligent exchange or dosing units the cylinder volume is checked. At the start of the dosing the validity of the titer and the expiry date of the selected standard will be checked as well as the GLP test interval for the exchange or dosing unit. The titer (Variable TITER) and the concentration (Variable CONC) are also available for calculation (CALC command, see *Section 4.5.1*).

- **Dosing rate:** Three predefined sets of parameters can be selected for the dosing rate.

With **slow** the dosing rate is at 10 % of the maximum dosing rate.

With **medium** the dosing rate is at 50 % of the maximum dosing rate.

With **fast** the dosing rate is equivalent to the maximum dosing rate.

The maximum dosing rate depends on the cylinder volume of the exchange or dosing unit used (see *Section 3.8.6*).

- **Delta U:** This input field is only editable with the addition method "auto". The individual addition increments are calculated and added in such a way that this constant potential difference is achieved.

Addition increments

The volume of the individual increments is defined under **Addition increments**:

- **Volume:** Volume that is added in each addition step.
- **Take over current value or all:** If this checkbox is activated, the volume entered for the first increment is adopted for all increments.



Note!

The sample size must be entered in mL for the correct calculation of the concentration.

The parameters for **Control device**, **Sensor** and **Stirrer** are described in *Section 4.1.5*. The selection of the **Direct parameters** is carried out as described in *Section 4.1.6*.

4.3 Measurements (MEAS Cond)

Measuring parameters

The parameters for the measurement sequence are edited under **Measuring parameters**.

- **Signal drift (d)**: Drift, i.e. the alteration in the measured value per minute that has to be reached for measured value acceptance. **off** means that the measured value acceptance takes place when the maximum waiting time has elapsed. This may be advisable if the electrode has a very slow response.



Note!

A **constant measured value** is often only achieved after a certain time, as mixing and possibly the reaction itself require a certain time. The response time of an electrode can also increase with time, i.e. reaching a constant measured value takes longer and longer. In such a case **drift-controlled measured value acceptance** is particularly advisable, as the measured values are only accepted when equilibrium has almost been achieved.

- **Waiting time min. (d)**: The measured value is not accepted until the minimum waiting time has elapsed, even if the measured value drift has already been reached. The minimum waiting time is only important for drift-controlled measurements.
- **Waiting time max. (d)**: If the signal drift is switched off or has not yet been reached then the measured value will be accepted after the maximum waiting time has elapsed.
- **Stop measured value (d)**: Stops when the preset measured value has been reached since the start of the measurement.
- **Time interval MP (d)**: Time interval for entering a measuring point in the list of measuring points. This list can contain max. 1000 measuring points.

Temp.
compens.

Editing the parameters for the **temperature compensation**:

- **Measuring temp. (d)**: Manually entered measuring temperature. If a temperature sensor is connected and temperature measurement is set to **automatic** or **continuous** under **Sensor** (see Section 4.1.5) then the temperature will be measured continuously.
- **Reference temp. (d)**: The measured conductivity is converted to this temperature.
- **Temp. coefficient (d)**: The temperature coefficient is required for converting the measured conductivity to the reference temperature.

The parameters for **Control device**, **Sensor** and **Stirrer** are described in Section 4.1.5. The selection of the **Direct parameters** is carried out as described in Section 4.1.6.

4.4 Evaluation

A list of measuring points can have various **additional evaluations** applied to it. The evaluation (**EVAL command**) always refers to the last titration or measurement in the method sequence. Which evaluations can be used for which titrations and measurements is given in the following table:

<i>Evaluation</i> <i>Titration</i> <i>Measurement</i>	<i>EVAL Fix-EP</i> <i>Fixed end-</i> <i>points</i>	<i>EVAL pK/HNP</i> <i>pK value</i> <i>Half neutraliza-</i> <i>tion potential</i>	<i>EVAL MIN/MAX</i> <i>Minimum/</i> <i>Maximum</i>	<i>EVAL BREAK</i> <i>Break points</i>	<i>EVAL RATE</i> <i>Rate evaluation</i>
<i>DET pH</i>	V, MV, t	pK value	yes	yes	–
<i>DET U</i>	V, MV, t	HNP	yes	yes	–
<i>DET Ipol</i>	V, MV, t	–	yes	yes	–
<i>DET Upol</i>	V, MV, t	–	yes	yes	–
<i>MET pH</i>	V, MV, t	pK value	yes	yes	–
<i>MET U</i>	V, MV, t	HNP	yes	yes	–
<i>MET Ipol</i>	V, MV, t	–	yes	yes	–
<i>MET Upol</i>	V, MV, t	–	yes	yes	–
<i>SET pH</i>	V, MV, t	–	yes	–	yes
<i>SET U</i>	V, MV, t	–	yes	–	yes
<i>SET Ipol</i>	V, MV, t	–	yes	–	yes
<i>SET Upol</i>	V, MV, t	–	yes	–	yes
<i>KFT Ipol</i>	V, MV, t	–	yes	–	yes
<i>KFT Upol</i>	V, MV, t	–	yes	–	yes
<i>STAT pH</i>	V, MV, t	–	yes	–	yes
<i>STAT U</i>	V, MV, t	–	yes	–	yes
<i>MEAS pH</i>	MV, t	–	yes	yes	–
<i>MEAS U</i>	MV, t	–	yes	yes	–
<i>MEAS T</i>	MV, t	–	yes	yes	–
<i>MEAS Ipol</i>	MV, t	–	yes	yes	–
<i>MEAS Upol</i>	MV, t	–	yes	yes	–
<i>MEAS Conc</i>	–	–	–	–	–
<i>MEAS Cond</i>	MV, t	–	yes	yes	–

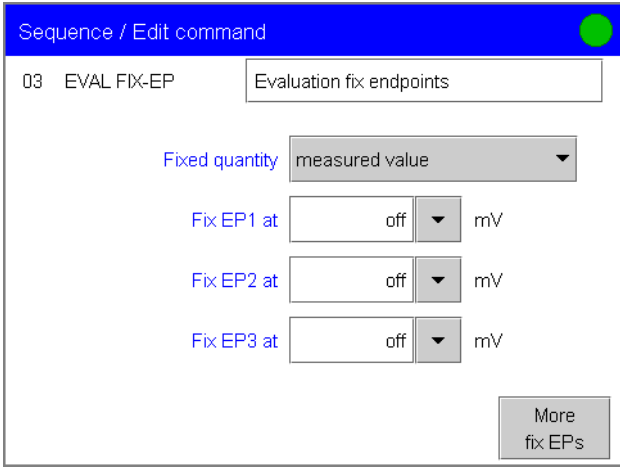
Only those evaluations which are available for the last titration or measurement before the EVAL command can be inserted in the list of commands. If a titration or measurement is deleted before the EVAL com-

mand then it will be shown in red in the list of commands, as the reference is missing.

You can also insert EVAL commands in the method sequence at a later date and trigger the **re-evaluation** under **Results** with **[Recalculate]**. The data for each evaluation can be shown under **Results/More determination data/View data** and can be calculated in CALC commands.

4.4.1 Evaluation of fixed endpoints (EVAL FIX EP)

Fixed endpoints can be determined for all titrations and measurements (except MEAS Conc). For a fixed quantity (measured value, volume or time) the associated values are interpolated from the list of measuring points.



Sequence / Edit command

03 EVAL FIX-EP Evaluation fix endpoints

Fixed quantity measured value

Fix EP1 at off mV

Fix EP2 at off mV

Fix EP3 at off mV

More fix EPs

- **Fixed quantity:** Selection of the fixed quantity.
- **Fix EP1 at** to **Fix EP9 at:** For the entered measured value, volume or time the associated values for the other quantities are interpolated from the list of measuring points. The fixed EP must lie between the first and last entries in the list of measuring points.

Up to nine fixed endpoints can be evaluated for each **EVAL FIX EP**.

4.4.2 Evaluation of pK value and half neutralization potential (EVAL pK/HNP)

The pK value can be determined for pH titrations (DET and MET) and the half neutralization potential can be determined for U titrations.

The activities of conjugated acid-base pairs are linked by the following equation (Henderson-Hasselbalch equation):

$$\text{pH} = \text{pK}_a + \log (a_B/a_A)$$

If the activities of the acid and the conjugated base are equal ($a_A = a_B$), then $\text{pH} = \text{pK}_a$. This is the value at the half neutralization point and can be extrapolated from the titration curve. A careful pH calibration is necessary for pK evaluations and even then the determined pK value is only an approximation, as the ionic strengths are not taken into account. In order to obtain a more accurate value, titrations must be carried out with decreasing ionic strengths and the results extrapolated to the ionic strength zero. pK evaluation in aqueous solution is limited to the range $3.5 < \text{pK} < 10.5$ because of the leveling effect of strong acids and the lack of jumps with very weak acids. pK values of mixtures of acids and polyvalent acids can also be determined.

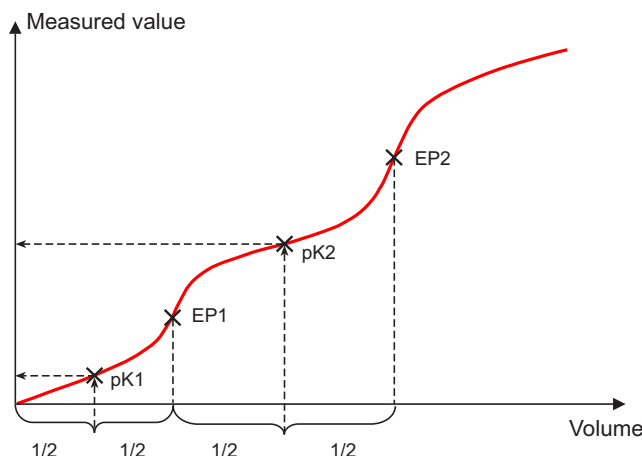


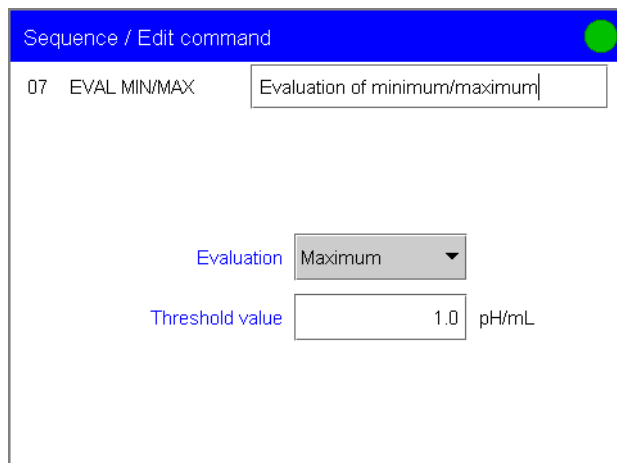
Fig. 4.15: Determining the pK value from the titration curve

In non-aqueous solutions the half neutralization potential (HNP) is frequently used instead of the pK value. The HNP is evaluated in the same way as the pK value.

No parameters can be edited for the command EVAL pK/HNP. If a start volume is to be added then it must be smaller than $1/2 V_{EP1}$.

4.4.3 Evaluation of minimum and maximum (EVAL MIN/MAX)

For the minimum or maximum measured value the associated volume, time and temperature are interpolated from the list of measuring points. The evaluation begins as soon as the slope of the curve exceeds a particular threshold value.



- **Evaluation:** In an EVAL MIN/MAX command either the minimum or the maximum can be evaluated. If you require both values then you must define a second EVAL MIN/MAX command in the method sequence.
- **Threshold value:** The evaluation begins as soon as the slope of the curve exceeds the set threshold value. Use a lower threshold value if the minimum or maximum is not found.

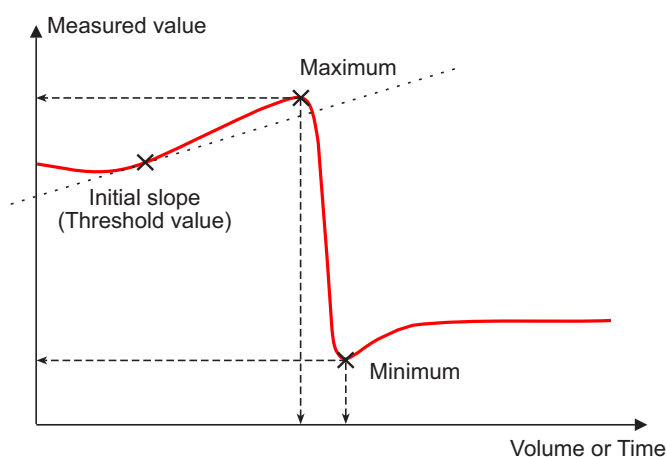


Fig. 4.16: Evaluation of minimum and maximum

4.4.4 Evaluation of break points (EVAL BREAK)

A break point evaluation is used to determine sharp change of direction in the titration curve. This evaluation is primarily used for photometric and conductivity titrations. The method is based on the search for extremes in the second derivative of the curve.

Sequence / Edit command

03 EVAL BREAK Break point evaluation

EP criterion 0.3

Slope 0.9

Smoothing factor 5

Set windows off

Set window

- **EP criterion:** Measure for the minimum sharpness of the break. The smaller the EP criterion set, the more break points will be found. As this is a relative value related to the total measured value alteration, even small changes in the measured value can be evaluated as a break point for a small measured value range.
- **Slope:** Minimum difference between the slope before and after the breakpoint. The smaller the difference, the more breakpoints will be found.
- **Smoothing factor:** The higher the smoothing factor, the fewer breakpoints will be found.
- **Set windows:** A range (window) can be defined on the measured value axis, on the volume axis or on the time axis. The breakpoint evaluation will only be carried out in the defined window. Only the first breakpoint in the defined window will be recognized.

[Set window] opens the dialog for entering the upper and lower limits.

- **Lower limit:** Measured value, time, or volume for the lower limit of the window.
- **Upper limit:** Measured value, time, or volume for the upper limit of the window.

All calculable variables can also be applied as result variable R1...R9. That means that you have to define the results in a preceding CALC command.

It is also possible to evaluate several breakpoints in a single window.

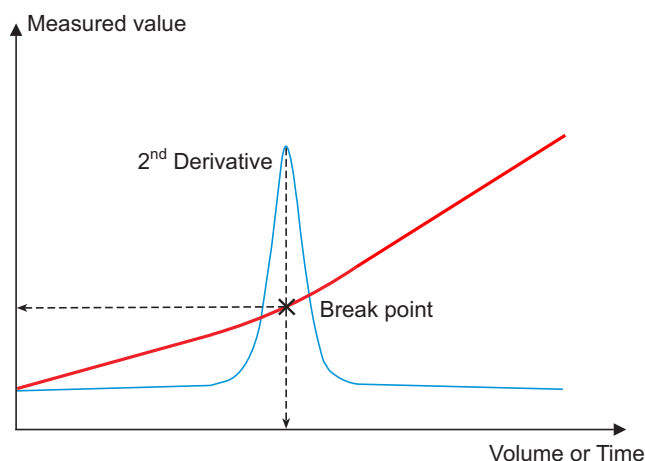


Fig. 4.17: Evaluating a breakpoint

4.4.5 Rate evaluation (EVAL RATE)

The rate evaluation produces the average dosing rate in a defined range (so-called window).

The average dosing rate is determined by linear regression using at least three measuring points. If dosing is carried out with one dosing device only and more than one cylinder volume is dosed then the average dosing rate will be reduced because of the filling time.

When the command is opened for the first time you will see that it already contains a window which covers the whole time range. You can add and edit new windows with **[New]**. Up to nine windows can be defined. The selected window can be removed from the list with **[Delete]**. You can use **[Edit]** to adapt the upper and lower limits for the selected window.

Edit command / Edit ●

03 EVAL RATE Rate evaluation

Lower limit 1 s

Upper limit 1 s

- **Lower limit #:** Time for the lower limit of the window.
- **Upper limit #:** Time for the upper limit of the window.

All calculable variables can also be applied as result variable R1...R9. That means that you have to define the results in a preceding CALC command. In contrast to a DET/MET titration the individual windows may overlap each other.

If the limit value is between two entries of the measuring point list then the next measuring point outside the window is included in the calculation.

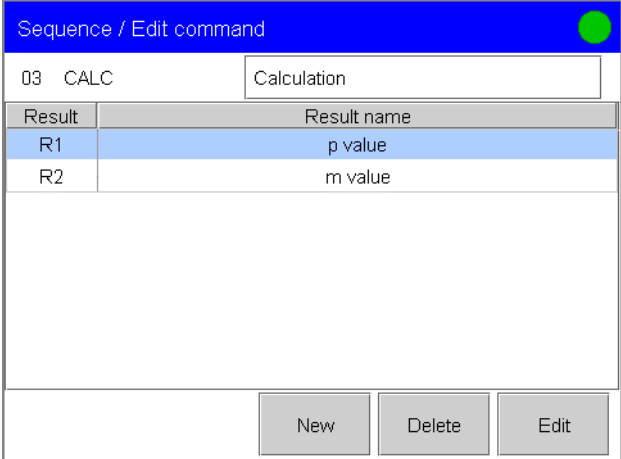
4.5 Calculations

In the method sequence **result calculations** can be defined with the CALC command. A method can contain a maximum of nine CALC commands each with nine result calculations. The CALC commands also contain instructions for statistical calculations, titer assignments, storing common variables and storing results in the result silo. Limits can also be defined for the results. A range of calculable **variables** (raw data from the determination, previously calculated results and system-specific variables) is available for the calculations. Results which are calculated in the method sequence can be entered as variables for parameters.

During titrating or measuring a calculated result can be displayed live with the CALC LIVE command. The current volume or measured value respectively is calculated for this purpose. This is helpful e. g. for KF titrations in order to follow the water content during the titration.

4.5.1 CALC command

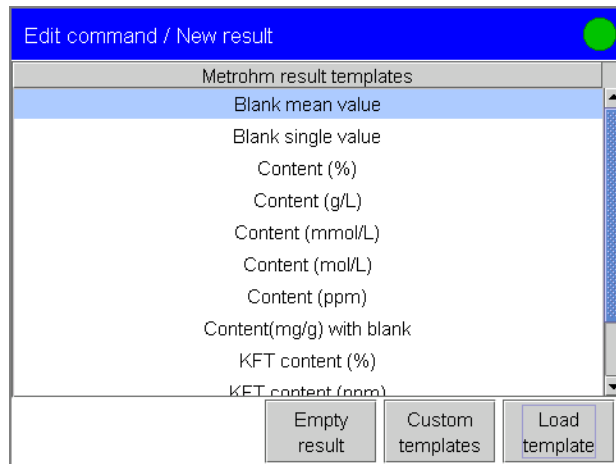
Up to nine result calculations can be defined in a CALC command. The results will be calculated in the sequence which is defined by the numbering of the result variables: R1...R9.



Result	Result name
R1	p value
R2	m value

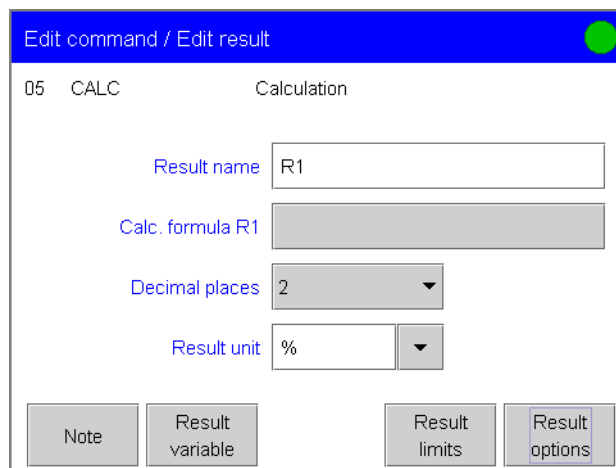
In the list of results you can use **[Edit]** to enter the equations and parameters for the result calculation and delete the selected result with **[Delete]**.

☞ You can insert a new result calculation in the list with **[New]**. The list with Metrohm result templates is opened.

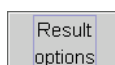


The result template chosen in the selection list is loaded with **[Load template]** and a note concerning the template is shown. With **[Custom templates]** you can open the list of your own result templates (see *Section 3.14.3*, *Section 4.5.4* and *Section 4.5.5*).

☞ Use **[Empty result]** to open the edit dialog directly.



- **Result name:** The standard result name corresponds to the result variable. The result name is the text which will be shown in the result display and in the report. It can be altered at any time.
- **Calculation formula:** The result variable is shown before the calculation formula. The variable can be altered under **[Result variable]**. A special editor is opened for the calculation formula if you touch the input field or click on it (see *Section 4.5.3*).
- **Decimal places:** Number of decimals to be shown in the result.
- **Result unit:** The result unit is shown and saved together with the result.



Under **Result options** various parameters for the result calculation can be edited:

- **Variable for mean:** If **statistical calculations** has been switched on for the method under **Sequence/ Method options** then the mean value of the individual results will be stored as the variable **SMNx** (x = 1 to 9). Statistical calculations can be carried out for up to nine results in one determination. The first free statistics variable will

always be shown as the default value. If no mean value is to be calculated for a result this variable should be set to **off**. The mean value for the result can be accessed via the statistics variable for further calculations.

- **Save result as titer:** The result can be saved as a titer. The titer is assigned to the titrant defined in the last titration command before the calculation. Please note that the CALC command containing the titer assignment is inserted after the titration command with which the titer is determined. If the **titer determination** is a single determination then you should select **Single value**. If a multiple determination is carried out then select **Mean value**. When the titer is assigned it will also be entered in the **History** (see *Section 3.8.4*). If a mean value is assigned then the last history entry will always be overwritten by the current mean value until all the determinations in the statistics series have been carried out. This means that there is only one history entry for a multiple determination. If single values are assigned then, when a determination is recalculated, the last entry will only be overwritten when it is the same determination that is being recalculated.
- **Save result as common variable:** The calculated result can be saved as an **instrument-specific common variable**. It is then also available in other methods for calculations. Even if statistics is switched on it is always the single value that is saved.
- **Variable:** Selection of the common variables to be assigned to the result. Result name, value and unit are entered in the list of common variables.
- **Display result:** The **intermediate results** display can be switched off. The result will then no longer be shown in the result dialog, nor will it be printed out in the result report.
- **Save result in result silo:** In the **result silo** you can save results which have been obtained by using different methods. This may be advisable when, for instance, the results of all determinations carried out on a particular day are to be shown clearly. Nine results from a single determination can be stored in the result silo.
- **Precision:** Setting which determines the **accuracy** with which the result is to be further calculated. The result can be rounded off to the number of **decimal places** defined under **Edit result**, cut off after this number of decimal places or calculated with the full accuracy of the floating point number ("double precision" to Standard IEEE 754).

Result
limits

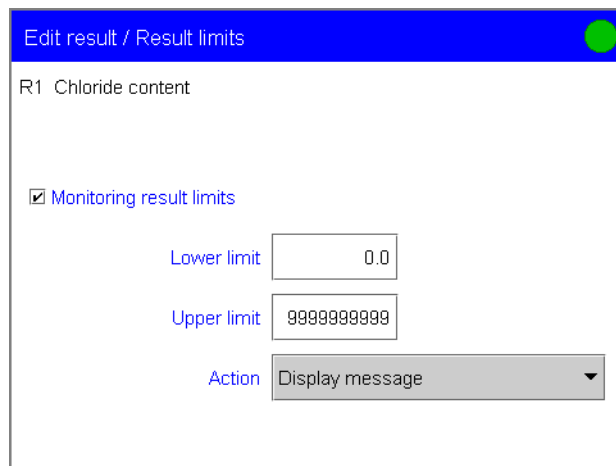
Limits can be defined for each result to be calculated. These **Result Limits** are monitored in the determination sequence when the calculation is carried out. If the result limits are monitored and remain within the limits then the result will be shown **green** in the result display; if the limits have been infringed then it will be shown in **red**.



Note!

Assigning a result to a titer or a common variable is only possible if the result is within the limits defined here.

☞ Open the dialog **Edit result/Result limits** and activate the **Monitoring result limits** checkbox.



☞ Enter an **Upper limit** and a **Lower limit** for the result. If a result is invalid then it will be treated as if the limits had been infringed.

The following **actions** are available if the result limits are infringed:

- **Display message:** The run is halted and a message is shown. You can choose whether you want to terminate the run or continue with it. The message will be documented under **Results/More determination data/Messages**.
- **Document message:** The run is not halted. A message that the result limits have been infringed will be documented under **Results/More determination data/Messages**.
- **Cancel determination:** The run is terminated and a corresponding message will be displayed and documented under **Results/More determination data/Messages**.

Result variable

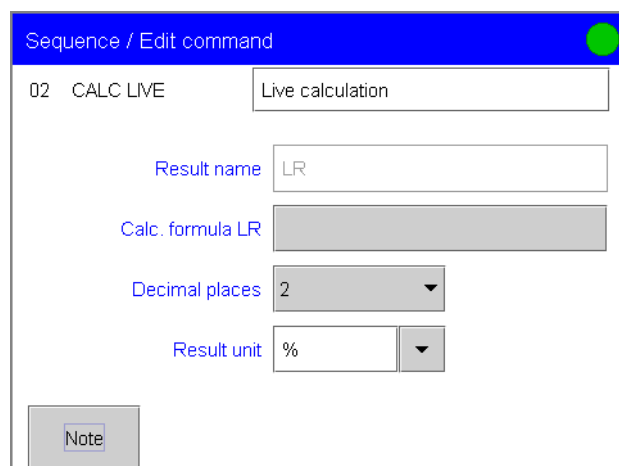
The **Result variable** is assigned automatically when a new result calculation is created. However, it can still be altered later. Only the result variables Rx (x = 1 to 9), which have not yet been assigned in this CALC command, can be selected. The value of the result can be accessed via the result variable. This means that a result can be used for further calculations.

Note

Under **Note** you can enter a short text, e. g. to describe the calculation variables used.

4.5.2 CALC LIVE command

The CALC LIVE command must be inserted directly before the corresponding titration or measuring command.



The CALC LIVE command is identical with the CALC command except for the following differences:

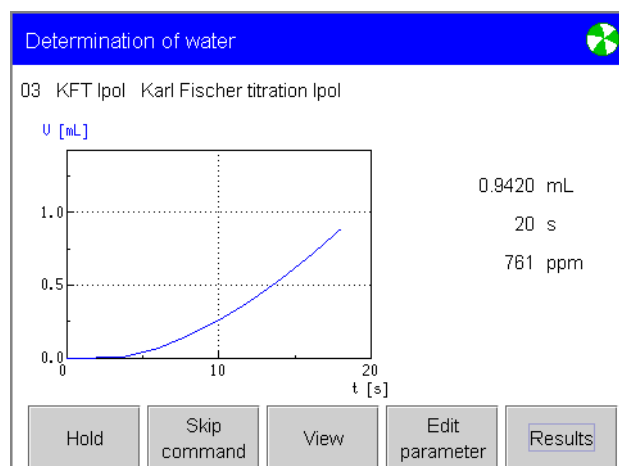
- The number of the variables which can be calculated is limited.
- No result options are available.
- The result cannot be monitored.
- The result variable cannot be altered.
- The live result is displayed only during a running titration or measurement. It appears neither in the result dialog nor in a report.

Entering the calculation formula is described in the following section.

Please proceed as follows for the live result to be displayed:

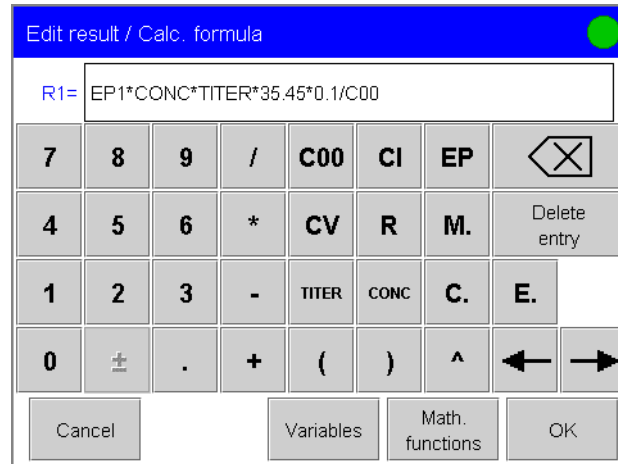
- ☞ Select the parameter **Live result** in the menu **View/Measured value options** (see Section 3.20.4).

The current result is now displayed in the live display:



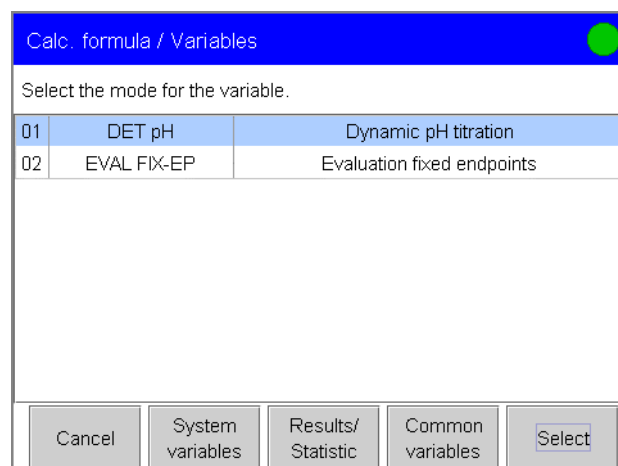
4.5.3 The formula editor

The formula editor is used to enter the **formulas for the result calculations**. The formula editor has an automatic **syntax check**, which is triggered when the formula is accepted. The priority rules which are normally valid apply to the calculation operations.



The **result variable** is shown in front of the input field. Buttons are available for entering numbers, mathematical operators and variables. The backspace key **[X]** deletes the character in front of the cursor. **[Delete entry]** will delete the whole formula. You can position the cursor within the formula by using the arrow keys. The maximum formula length is 100 characters.

You can use **[Variables]** to open selection lists for all the variables which are available. By selecting the variable from the list you can avoid syntax errors. If the method sequence contains several titrations, measurements or evaluations before the calculation then a selection list containing the corresponding commands will first be opened.



You can use **[Select]** to open the list of variables for the selected titration, measurement or evaluation. For example, if you select a titration in the DET mode, the list of variables will look like this:

Calc. formula / Variables	
Variable	Description
C00	Sample size
CI1	Sample identification 1
CI2	Sample identification 2
1M.TITER	Titer of selected titrant
1M.CONC	Concentration of selected titrant
1M.EP#	Endpoint volume for EP#
1M.MCV	End volume
1M.MCD	Total duration of mode
1M.MSV	Start volume (all start conditions)
1M.MIM	Initial measured value

Buttons: Cancel, Insert

The selected variable is entered in the formula with **[Insert]** or **[Back]**. With **[Cancel]** you can exit the list without accepting a variable. The individual variables are described in *Section 4.5.7*. The character **#** stands for a running number (usually from 1 to 9 or 10); this must be entered manually. If you want to calculate **EP1**, for example, then **EP** is inserted in the formula and you must enter the **1** in the formula editor.

If the method contains more than one data producing command before the calculation then the command identification will be given before the variables (e. g. **1M.TITER** for the titrant titer used in the first titration). Data concerning the titrations, measurements and calibrations have the identification **M** for mode; evaluation data have the identification **E** for evaluation; calculation data have the identification **C** for calculation. The command identification (M, E, C) will be counted up separately for each command type and does not necessarily correspond with the number of the command line.

[System variables] opens the list of system variables:

Variables / System variables	
Variable	Description
%RN	Sample number
%SC	Start counter
%AS	Autostart status
%AC	Autostart counter
%AD	Preset number of autostart counter
%SS	Sample data silo status
%SL	Current silo line
%SE	Silo end reached

Buttons: Cancel, Insert

[Results/Statistics] opens the list containing the existing results and the statistics variables:

If invalid variables (e. g. missing endpoints) could occur in a result calculation then these can be replaced with a valid value (replacement value) by using the **test function TST**. In this way invalid results can be avoided.

Syntax: TST (variable to be tested, replacement value)

4.5.4 Creating custom result templates

Under **System/Templates/Custom result templates** you can create templates for result calculations (see *Section 3.14.3*). These result templates can be used when editing a CALC command (see *Section 4.5.1* and *Section 4.5.5*).

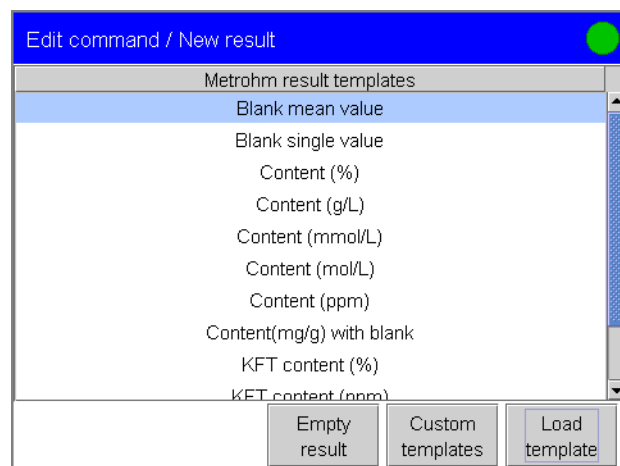
In principle, **creating result templates** works in the same way as editing a new result in the CALC command, except that no result variable can be assigned in the result template and no result limits can be defined. These are both carried out after the template has been loaded when editing the result calculation in the CALC command. The variables are also given without command identifications. If required, these must be entered in the CALC command.

In the calculation formulas you can use the **variables F1 to F9** as placeholders, e. g. for the molar mass. These F-variables are automatically requested after the display of the note when the result template is loaded.

Under **Note for wizard** you can enter a text in the result template which will be shown automatically when the result template is loaded before the F-variables are requested. If you do use F-variables in your templates then you should describe them in this note.

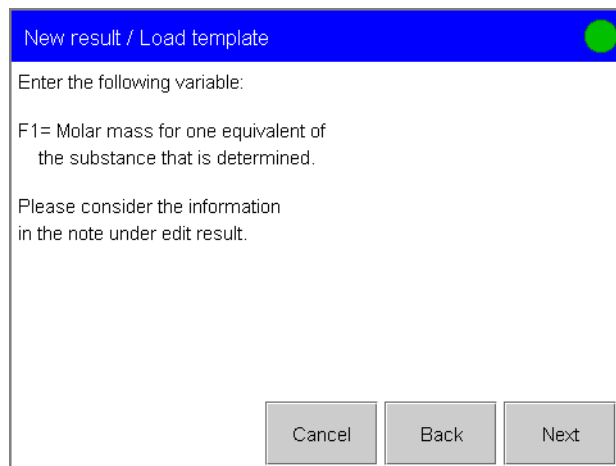
4.5.5 Loading result templates

Loading result templates takes place when new result calculations are defined in the CALC command.

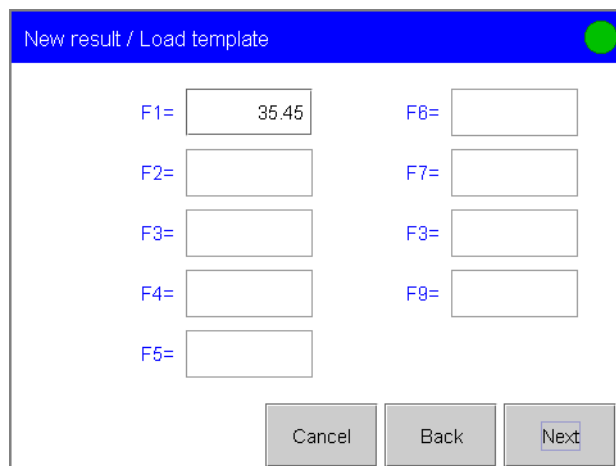


With **[Load template]** the result template selected in the selection list is loaded and the note for the template is shown. With **[Custom templates]** you can show the list of your own result templates (see *Section 3.14.3*).

☞ Select a result template from the list and load it with **[Load template]**.

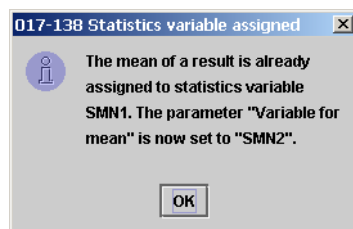


The **F-variables** used in the result template are automatically requested when the template is loaded if the display of the note is closed by pressing **[Next]**.



The only input fields which are active are those for the variables used in the result template. The entered values will be inserted automatically in the calculation formula in place of the variables.

If the mean value of a result is assigned to a variable SMNx (x = 1 to 9) in the result template and this has already been used in a different result calculation, then a message will appear to inform you that the next free variable will be used for the mean value assignment:



4.5.6 Conversion table of the calculating formula for KF titrations

$$\text{water content} = \frac{[\text{volume(KF - reagent)} - \text{blank}] \cdot \text{titer} \cdot \text{factor}}{\text{sample size} \cdot \text{divisor}}$$

Result unit	Sample size in...	Factor	Divisor
%	g	0.1	1
%	mg	100	1
%	mL	0.1	Density of sample in g/mL
ppm	g	1000	1
ppm	mL	1000	Density of sample in g/mL
ppm	µL	1	Density of sample in g/mL
mg/mL	g	Density of sample in g/mL	1
mg/mL	mL	1	1
mg	1	1	1
mL	1	1	Density of H ₂ O in mg/mL
mg/pc	pc	1	1

4.5.7 Calculable variables

The following table lists all those variables which can be used in calculations. When editing the formula you can either enter the variables directly or select them from the list of variables under **Calc. formula/Variables** and then insert them in the formula. For variables which contain an index (e. g. EP1) the index must be entered manually. The index is always given in the selection list as #.

If the method sequence contains more than one data producing command (titrations, measurements, calibrations, monitored dosing, evaluations, calculations) before the calculation then you can insert the command identification by using the following buttons in the formula editor: 'M.' (titration or measuring mode or monitored dosing), 'E.' (EVAL) and 'C.' (CALC). You must enter the index for the command in front of the letter. If the variables are entered without command identification then the variables from the last command before the CALC command to provide the corresponding variables will always be used. A safer method is to insert the variables from the list of variables, as only the variables produced in the determination are available. The vari-

ables with the necessary command identifications are shown in the list of variables.


Attention!

If you subsequently enter commands in the list of commands, then the **command identifications** of the variables in the calculations will not be adapted automatically.

	<i>Variable</i>	<i>Description</i>	<i>Method command</i>
Sample data	COO	Sample weight	all
	CI1 CI2	Sample identification 1 and sample identification 2 The sample identifications can be used in calculations if numerical values are entered.	all
Determination	DD	Duration of determination (see Section 3.18.4) Time between the START of the determination and the normal end of the run or manual termination with [STOP] . If the determination is not yet finished then the time between the start and the use of the variable in the CALC command will be used.	all
Titrant	TITER	Titer of the titrant selected in the titration command	DET, MET, SET, KFT, STAT, DOS
	CONC	Concentration of the titrant selected in the titration command	DET, MET, SET, KFT, STAT, DOS
Titrations, measurements, calibrations	EP#	Equivalence point (DET and MET) or end-point volume (SET, KFT) for EP#	DET, MET, SET, KFT
	EM#	Equivalence point (DET and MET) or end-point measured value (SET, KFT) for EP#	DET, MET, SET, KFT
	EF#	Equivalence point ERC for EP#	DET, MET
	ET#	Equivalence point (DET and MET) or end-point temperature (SET, KFT) for EP#	DET, MET, SET, KFT
	ED#	Equivalence point (DET and MET) or end-point time (SET, KFT) for EP#	DET, MET, SET, KFT
	ESI#	Equivalence point marking (0 if one EP in window, 1 if more than one EP in window)	DET, MET
	MIM	Initial measured value (measured value before start conditions are processed)	DET, MET, SET, KFT, STAT, MEAS, DOS

	<i>Variable</i>	<i>Description</i>	<i>Method command</i>
	MIT	Initial temperature (temperature before start conditions are processed)	DET, MET, SET, KFT, STAT, MEAS, DOS
	MSA	Start volume which is added according to the start volume given in the start conditions.	DET, MET
	MSP	Start volume which is added according to the start measured value given in the start conditions.	DET, MET
	MSS	Start volume which is added according to the start slope given in the start conditions.	DET, MET
	MSV	Start volume for all start conditions (start volume, start measured value and start slope)	DET, MET, SET, KFT, STAT
	MSD	Time for processing the start conditions	DET, MET, SET, KFT, STAT
	MSM	Start measured value (measured value after processing the start conditions)	DET, MET, SET, KFT, STAT, DOS
	MST	Start temperature (temperature after processing the start conditions)	DET, MET, SET, KFT, STAT, DOS
	MCV	End volume (total volume added at end of titration)	DET, MET, SET, KFT, STAT, MEAS Conc, DOS
	MCD	Total duration of titration, measurement or calibration (including start conditions)	DET, MET, SET, KFT, STAT, MEAS, DOS, CAL
	MTM	Method of temperature measurement (Pt1000, NTC, manual); format = text	DET, MET, SET, KFT, STAT, MEAS, DOS
	MDD	Duration of net dosing (without filling times, pause)	DOS
	MDC	Drift for drift correction	SET, KFT
	DDC	Time for drift correction	SET, KFT
	MCM	Final measured value (measured value at end of the titration or measurement); MEAS: corresponds to the measured content	DET, MET, SET, KFT, STAT, MEAS, DOS
	MCT	Final temperature (temperature at end of the titration, measurement or calibration)	DET, MET, SET, KFT, STAT, MEAS, DOS, CAL

	<i>Variable</i>	<i>Description</i>	<i>Method command</i>
	MMP	Number of measuring points in the list of measuring points	DET, MET, SET, KFT, STAT, MEAS, DOS
	MTS	Stop type (termination of the titration, measurement or calibration), format: text	DET, MET, SET, KFT, STAT, MEAS, DOS, CAL
Sensor	MEN	Electrode zero point pH(0) or E(0)	DET, MET, SET, KFT, STAT, MEAS, DOS, CAL
	MSL	Slope of electrode	DET, MET, SET, KFT, STAT, MEAS, DOS, CAL
	MVA	Variance of electrode (mathematically only defined for three standards or more); CAL Conc: calculated only if calibration is carried out with a minimum of four standards	MEAS Conc, CAL Conc
Evaluation fixed endpoints	FP#	Fixed endpoint volume for FP#	EVAL FIX-EP
	FM#	Fixed endpoint measured value for FP#	EVAL FIX-EP
	FT#	Fixed endpoint temperature for FP#	EVAL FIX-EP
	FD#	Fixed endpoint time for FP#	EVAL FIX-EP
Evaluation pK value / half neutralization potential	HP#	pK/HNP volume for HM#	EVAL pK/HNP
	HM#	PK value, or half neutralization potential	EVAL pK/HNP
	HT#	pK/HNP temperature for HM#	EVAL pK/HNP
	HD#	pK/HNP time for HM#	EVAL pK/HNP
Evaluation minimum	XIP	Volume to minimum measured value	EVAL MIN/MAX
	XIM	Minimum measured value	EVAL MIN/MAX
	XIT	Temperature to minimum measured value	EVAL MIN/MAX
	XID	Time to minimum measured value	EVAL MIN/MAX
Evaluation maximum	XAP	Volume to maximum measured value	EVAL MIN/MAX
	XAM	Maximum measured value	EVAL MIN/MAX
	XAT	Temperature to maximum measured value	EVAL MIN/MAX
	XAD	Time to maximum measured value	EVAL MIN/MAX
Evaluation break point	BP#	Breakpoint volume for BP#	EVAL BREAK
	BM#	Breakpoint measured value for BP#	EVAL BREAK
	BT#	Breakpoint temperature for BP#	EVAL BREAK
	BD#	Breakpoint time for BP#	EVAL BREAK

	<i>Variable</i>	<i>Description</i>	<i>Method command</i>
Evaluation rate	RD#	Mean rate for time slots	EVAL RATE
	RDS#	Standard deviation for RD#	EVAL RATE
	RDC#	Correlation coefficient for RD#	EVAL RATE
	RM	Mean rate for whole range	EVAL RATE
	RMS	Standard deviation for RM	EVAL RATE
	RMC	Correlation coefficient for RM	EVAL RATE
Results	R1 to R9	Results which can be calculated with a CALC command	CALC
Statistics	SMN#	Mean value #, the variables for the mean value are assigned under Result options (see <i>Section 4.5.1</i>).	CALC
	SSA#	Absolute standard deviation of SMN# (see <i>Section 3.21.1</i>)	CALC
	SSR#	Relative standard deviation of SMN# (see <i>Section 3.21.1</i>)	CALC
	SNR#	Number of results from the mean calculation (see <i>Section 3.21.1</i>)	CALC
	SSD	Preset number of determinations for the statistics (see <i>Section 3.16.4</i>)	CALC
	SNT	Statistics status (1 for statistics on, 0 for statistics off)	CALC
Common variables	CV01 to CV25	Instrument-specific common variables	
System variables	%RN	Sample number (see <i>Section 3.18.4</i>)	
	%SC	Start counter (see <i>Section 3.18.4</i>)	
	%AS	Autostart status (1 for autostart on, 0 for autostart off)	
	%AC	Actual autostart counter (see <i>Section 3.17.3</i>)	
	%AD	Preset number of autostarts (see <i>Section 3.17.3</i>)	
	%SS	Sample data silo status (1 for sample data silo on, 0 for sample data silo off)	
	%SL	No. of sample data silo lines that have been processed	
	%SE	End of sample data silo reached (1 for yes, 0 for no)	

4.5.8 Result variables as parameters

In many numerical entries for **method parameters** you can also enter a **result** which has previously been calculated (e. g. **R1**) instead of a number. The result must have been calculated in a previous CALC command in the method sequence. Please note that the result must be within the input limits for the parameter, as otherwise the determination run will be halted when the parameter is accessed.

With PC Control the result variables are entered directly via the PC keyboard. With Touch Control the button **[R1]** is used to open the numerical input dialog with a selection of result variables from R1 to R9 (see Section 3.1.4).

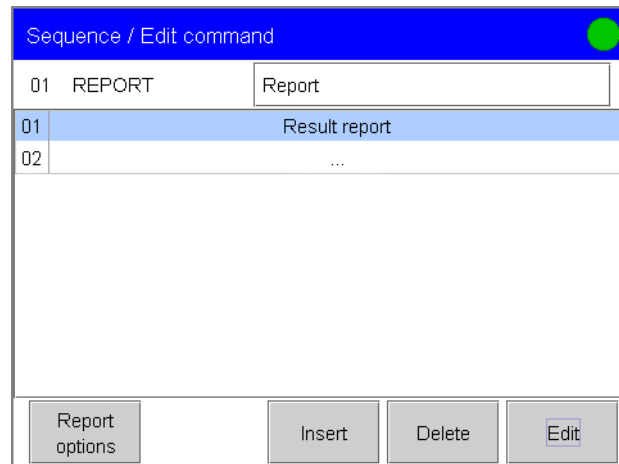
A typical application is the use of a **relative start volume**. To define a start volume which is dependent on the **sample weight** proceed as follows:

- ☞ Before the titration command define a **CALC command** in which the relative start volume is calculated, e. g. $R1 = C00 * 3$ (C00 = sample weight).

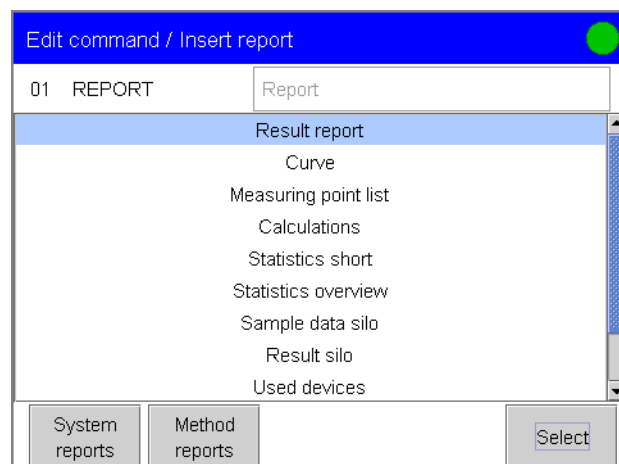
- ☞ In the **titration command** enter the variable R1 as the start volume.

4.6 Reports

In the **REPORT command** you can define a maximum of ten reports which can be printed out in the method sequence. The reports which are defined in a report command are printed out in the sequence in which they are entered in the list.



☞ You can insert a report in the list in front of the selected line with **[Insert]**.

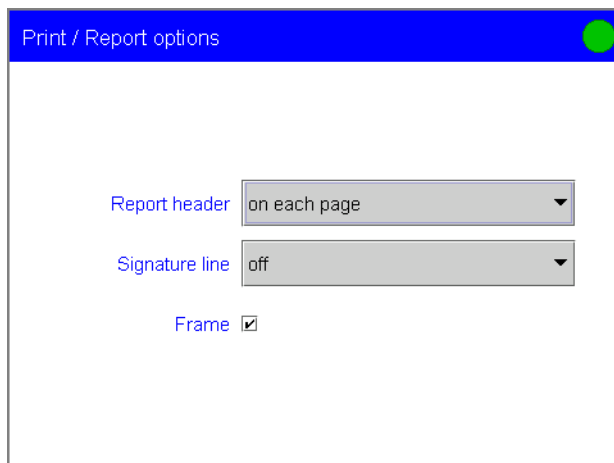


You can use **[Method reports]** to open the list of reports for the current method. **[System reports]** opens the list of reports for system-specific data.

☞ Mark the required report in the selection list and include it in the list of reports with **[Select]**.

In the list of reports you can use **[Delete]** to delete the selected report and **[Edit]** to edit the parameters for printing out the selected report.

☞ Open the dialog for the configuration of the whole report sequence with **[Report options]**.



In the **report header** the type, serial number and program version of the software (Touch Control or PC Control), the device name which you can enter in the device manager of Touch Control or PC Control and the printout date with time zone can be printed out. You can also define your own report header under **System/Templates/Report header**; this will be printed out before the standard report header (see *Section 3.14.7*). Under **Report header** you can choose whether the report header is to be printed out on every page, on the first page of the report only or not at all. The **Signature line** gives you the possibility of signing the report together with the date. You can choose whether the **Signature line** is to appear on every page, on the last page of the report only or not at all. If you have activated the **Frame** checkbox then a frame will be printed round each page of the report.

Parameters for the following reports can be edited in the method sequence:

	<i>Report</i>	<i>Parameter</i>
Results (current determination)	Result report	<ul style="list-style-type: none"> - Determination properties (on/off) - Sample data (on/off) - Sensor data for the sensor used (on/off) - Titrant data for the titrant used (on/off) - Raw data, i.e. equivalence points (DET, MET), endpoints (SET, KFT), control point (STAT), final measured values (MEAS), calibration data (CAL) and results of evaluations (EVAL) (on/off) - Used common variables (on/off) - Calculated results (on/off) - Statistics short (on/off) - Messages entered in the list of messages (on/off) - Lines between the sections (on/off)
	Curve	<ul style="list-style-type: none"> - Selection of the titration, measurement or calibration (mode) for which the curve is to be printed - Settings for the curve report (for a description of the settings see <i>Section 3.18.7</i>)

	<i>Report</i>	<i>Parameter</i>
	List of measuring points	- Selection of the titration or measurement (mode) for which the list of measuring points is to be printed out.
	Calculations	- Determination properties (on/off) - The variables can be printed out as shown or with the full accuracy of the floating point number ("double precision" to Standard IEEE 754).
	Devices used	Determination properties (on/off).
	Variables	All determination data; depends on command.
Statistics	Statistics short	Report printout at the end of a statistics series (statistic counter same as number of samples, i.e. samples processed = samples set) or at the end of each determination.
	Statistics overview	Report printout at the end of a statistics series (statistic counter same as number of samples, i.e. samples processed = samples set) or at the end of each determination.
Sample data	Sample data silo	Sample data silo properties, landscape format, Table with all the sample data that can be entered in the sample data silo.
Result silo	Result silo	Result data silo properties, landscape format, Table with all the results that can be stored in the result silo.
Form feed	Form feed	Not editable. Each report is printed out on a separate page.

No parameters can be edited for the system reports and the method reports. The contents of the individual reports is described in Section 3.23.



Note!

Some tables (*statistics overview and sample data silo*) are always printed out in **landscape format**, as otherwise the data could not be printed out on a single page. You must select **portrait** in the Windows-specific **Printer setting** nevertheless, as printout in landscape format is automatic.

4.7 Calibrating pH electrodes (CAL pH) and ISE (CAL Conc)

For **pH measurements**, titrations to a preset endpoint (SET pH) and the determination of pK values and fixed endpoints the calibration of the pH electrode (command CAL pH) is essential; it is also recommended for all other pH titrations. As least two buffers should be used for the calibration; these should cover the expected measuring range. For **concentration direct measurements** with ISE electrodes the sensor must be calibrated with a series of standards (CAL Conc). During the sequence the calibration data is stored automatically together with the sensor data for the used sensor.

Calibration parameters

Under **Calibration parameters** you can edit the parameters for the calibration sequence. These are identical for pH calibrations and ISE calibrations. In the command CAL pH you must define the calibration buffers, in the command CAL Conc the concentrations of the standards.

- **Signal drift (d)**: Drift, i.e. the alteration in the measured value per minute that has to be reached for measured value acceptance. **off** means that the measured value acceptance takes place when the maximum waiting time has elapsed. This may be advisable if the electrode has a very slow response.
- **Waiting time min. (d)**: The measured value is not accepted until the minimum waiting time has elapsed, even if the measured value drift has already been reached. The minimum waiting time is only important for drift-controlled measurements.
- **Waiting time max. (d)**: If the signal drift is switched off or has not yet been reached then the measured value will be accepted after the maximum waiting time has elapsed. If the waiting time has not been newly entered then a waiting time that is suitable for the drift will be calculated automatically according to the following equation:

$$\text{Waiting time} = 150 / \sqrt{\text{Drift} + 0.01} + 5$$

- **Temperature (d)**: Manually entered calibration temperature. If a temperature sensor is connected and temperature measurement is set to **automatic** or **continuous** under **Sensor** (see *Section 4.1.5*) then the temperature will be measured. If **off** is defined then the temperature is requested after the start (except the calibration is carried out with a Sample Processor).
- **Sample Processor (d)**: If the calibration is carried out with a Sample Processor then the buffers or standards are changed automatically. That is why there is no request of the calibration temperature at the start of the calibration. The value entered above is used.

For calibrations with a Sample Processor connected via a remote box the parameter **Remote** must be activated. When the measurement of a buffer or standard has been completed the Titrando sends a signal to the Sample Processor via the remote connection (EOD, see *Section 6.2.2*). The Sample Processor then switches to the next buffer or standard.

For automatic calibrations with the USB Sample Processor the parameter **USB** must be selected. The CAL command must be called up in a subsequence (see *Section 4.12.6*) with the subsequence option "**Cycles = Calibration**". In order to change the calibration solution a MOVE command (see *Section 4.12.1*) must be inserted before the CAL command with the target "**Calibration pos.**". The 1st calibration position must be defined in the rack table (see *Section 3.10.5*) as a sample position or as special beaker. If a sample position has been given as the 1st calibration position then it is essential that the other calibration solutions are placed in the directly following rack positions. If special beakers are used for the calibration then there must be as many special beakers defined as buffers or standard solutions are required for the calibration. The special beakers do not need to be placed in rack positions that directly follow each other.

Buffers

CAL pH only: The type and number of buffers used for calibration are entered under **Buffers**. Alternatively the pH values for a special buffer series can be entered.

- **Buffer type** (d): Selects a predefined buffer series for the calibration. The following buffer series are available: **Metrohm, NIST, DIN, Fisher, Fluka Basel, Mettler, Merck Titrisol, Beckman, Radiometer, Custom, Special, Merck CertiPUR, Baker, Hamilton, Precisa**. The temperature tables for the buffer series can be found in *Section 6.4*. If these buffers are used then the system will recognize them automatically. If you have defined your own series of buffers under **System/Templates/Custom calibration buffers** then select **Custom** in order to use them. Automatic buffer recognition will then be active for this series of buffers. You can also use **Special** to define up to five buffers directly in the calibration command. Automatic buffer recognition will then not be active and the buffers must be used for the calibration in the given sequence.
- **Number of buffers** (d): For predefined or custom buffer series: the number of buffers to be used for the calibration. If calibration is carried out without a Sample Processor then during the run the user will be requested to change the buffer for the required number of times. During calibration with a Sample Processor the buffers are changed automatically. If you use more than two buffers for your calibration then you can use a particular buffer several times in order to give it more statistical weight. The first two buffers must always be different.
- **Buffer 1 pH to Buffer 5 pH** (d): For buffer type **Special**: pH values of the buffers. Please note that you must enter the pH values corresponding to the measuring temperature used. **off** means that the buffer and all those following will not be used. During the sequence a message will appear the corresponding number of times to indicate the next buffer to be used.

Standards

CAL Conc only: Under **Standards** the concentration unit for the concentration measurements and the concentrations of the standard solutions are entered.

- **Unit Conc.** (d): Select the concentration unit of the standard. The concentration unit for concentration measurements always depends on the unit entered for the concentration of the standard.
- **Conc. standard 1 to Conc. standard 5** (d): Enter the concentration for 1 to 5 concentration standards. **off** means that the standard and all those following will not be used. During the sequence a message will appear the corresponding number of times to indicate the next standard to be used.

Stirrer control

Under **Stirrer control** you can edit the parameters for controlling the stirrer during the calibration. Take care that you have selected a stirrer under **Edit command/Stirrer**.

- **Stir solution during measurement** (d): Automatically switches the stirrer on/off at the start and the end of the measurement.
- **Stir before meas.** (d): If stirring is switched off during the measurement, the solution can be stirred before the measurement. Enter the corresponding time here.
- **Pause before meas.** (d): If stirring is carried out before the measurement, a pause interval can be entered here. No stirring or measuring occurs during this time.

The parameters for **Control device**, **Sensor** and **Stirrer** are described in Section 4.1.5.



Note!

Make sure that the sensor to be calibrated has been selected under **Edit command/Sensor**. This is the only way to ensure that the **calibration data** for this sensor is stored in the correct place under **System/Sensors**.

The choice of the **Direct parameters** is described in Section 4.1.6.

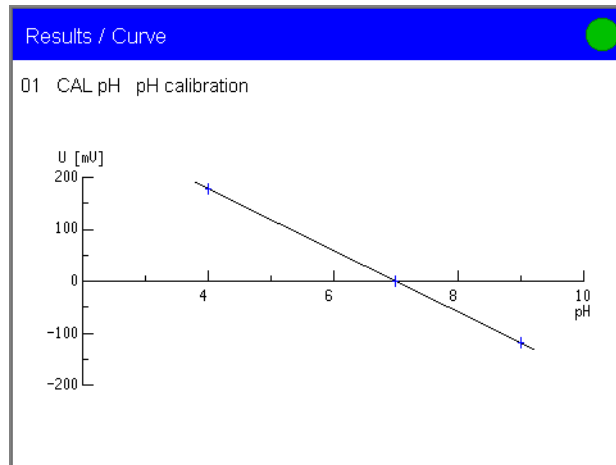
2-Point calibration with automatic buffer recognition

Immerse electrode in first buffer	With automatic buffer recognition the order of the buffers does not matter.
Start the calibration command	
Measure or enter the calibration temperature	If a temperature sensor is connected then the temperature will be measured. Otherwise a query will appear and the temperature must be entered manually.
(Stir and/or pause before measurement)	The solution is stirred before the measurement. Pause will be allowed to elapse before the measurement.

(Switch on stirrer)	The stirrer will be switched on if Stir solution during measurement is activated.
Measure buffer 1	The potential of buffer 1 is measured.
(Switch off stirrer)	The stirrer will be switched off if the buffer has been recognized and if Stir solution during measurement is activated.
Message showing which buffer has been recognized.	A message will be shown with instructions for the next buffer. When the electrode has been immersed in the second buffer the second measurement is started with [OK] .
(Stir and/or pause before measurement)	The solution is stirred before the measurement. Pause will be allowed to elapse before the measurement.
(Switch on stirrer)	The stirrer will be switched on if Stir solution during measurement is activated.
Measure buffer 2	The potential of buffer 2 is measured.
(Switch off stirrer)	The stirrer will be switched off if the buffer has been recognized and if Stir solution during measurement is activated.
Calculate calibration data	The calibration data, i.e. the slope and the electrode zero point pH(0) are calculated, the limits checked and, if necessary, an appropriate message displayed. The calibration data will be added to the sensor data for the particular sensor.

Optional steps are shown in brackets.

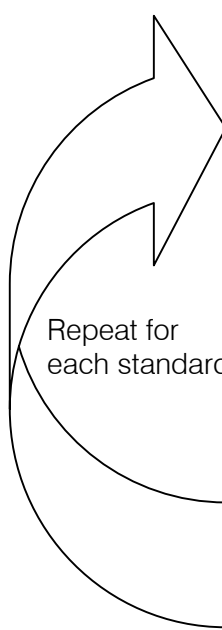
At the end of the determination sequence the calibration data is shown on the result page. The calibration curve is shown under **Results/Curve**:



The individual measured values for all buffers are shown under **Results/More determination data/View data**:

More determination data / View data				
01 CAL pH pH calibration				1M
Stop criterion	Regular stop			MTS
Calibration duration	42.8 s			MCD
Temp. measurement	manual			MTM
Calibration temp.	25.0 °C			MCT
pH(0)	6.998			MEN
Slope	100.1 %			MSL
	pH	U [mV]	T [°C]	t [s]
Buffer 1	9.000	-118.3	25.0	10
Buffer 2	7.000	-0.6	25.0	10
Buffer 3	4.000	177.6	25.0	10

Concentration calibration with up to 5 standards

	Immerse electrode in first standard	
	Start the calibration command	
	Measure or enter the calibration temperature	If a temperature sensor is connected then the temperature will be measured. Otherwise a query will appear and the temperature must be entered manually.
 <p>Repeat for each standard</p>	Message	A message appears with instructions for the first standard. Start the measurement with [OK] .
	(Stir and/or pause before measurement)	The solution is stirred before the measurement. Pause will be allowed to elapse before the measurement.
	(Switch on stirrer)	The stirrer will be switched on if Stir solution during measurement is activated.
	Measure standard	The potential of the standard is measured.
	(Switch off stirrer)	The stirrer will be switched off if the measured value has been accepted and if Stir solution during measurement is activated.
	Calculate calibration data	The calibration data, i.e. the slope, electrode zero point E(0) and the blank concentration c(blank) are calculated, the limits checked and, if necessary, an appropriate message displayed. The calibration data will be added to the sensor data for the particular sensor.

Optional steps are shown in brackets.

4.8 Calibrating conductivity measuring cells (CAL Cond)

The cell constant of a conductivity measuring cell can be determined with the CAL Cond command.

Calibration parameters

Under **Calibration parameters** you can edit the parameters for the calibration sequence.

- **Signal drift (d)**: Drift, i.e. the alteration in the measured value per minute that has to be reached for measured value acceptance. **off** means that the measured value acceptance takes place when the maximum waiting time has elapsed. This may be advisable if the measuring cell has a very slow response.
- **Waiting time min. (d)**: The measured value is not accepted until the minimum waiting time has elapsed, even if the measured value drift has already been reached. The minimum waiting time is only important for drift-controlled measurements.
- **Waiting time max. (d)**: If the signal drift is switched off or has not yet been reached then the measured value will be accepted after the maximum waiting time has elapsed.
- **Measuring temp. (d)**: Manually entered measuring temperature. If a temperature sensor is connected and temperature measurement is set to **automatic** or **continuous** under **Sensor** (see Section 4.1.5) then the temperature will be measured. If **off** is defined then the temperature is requested after the start.

Standard

Under **Standard** the characteristics of the calibration standard are entered. These values are proposed in the query after the start of the method.

- **Request at calibration start**: If this parameter is switched on then you are requested – after the start of the method – to enter the following parameters.
- **Conductivity std. (d)**: Enter the conductivity of the calibration standard used.
- **Reference temp. std. (d)**: Enter the reference temperature at which the calibration standard has the conductivity entered above.
- **Temp. coefficient (d)**: Enter the temperature coefficient corresponding to the above reference temperature.

Stirrer control

Under **Stirrer control** you can edit the parameters for controlling the stirrer during the calibration. Take care that you have selected a stirrer under **Edit command/Stirrer**.

- **Stir solution during measurement (d)**: Automatically switches the stirrer on/off at the start and the end of the measurement.
- **Stir before meas. (d)**: If stirring is switched off during the measurement, the solution can be stirred before the measurement. Enter the corresponding time here.
- **Pause before meas. (d)**: If stirring is carried out before the measurement, a pause interval can be entered here. No stirring or measuring occurs during this time.

The parameters for **Control device**, **Sensor** and **Stirrer** are described in *Section 4.1.5*.



Note!
 Make sure that the sensor to be calibrated has been selected under **Edit command/Sensor**. This is the only way to ensure that the **calibration data** for this sensor is stored in the correct place under **System/Sensors**.

The choice of the **Direct parameters** is described in *Section 4.1.6*.

Sequence of the cell constant determination

Immerse measuring cell in standard	
Start the calibration command	
Measure or enter the calibration temperature	If a temperature sensor is connected then the temperature will be measured. Otherwise a query will appear and the temperature must be entered manually.
(Enter data of standard)	The characteristics of the calibration standard are queried, if Request at calibration start is activated.
(Stir and/or pause before measurement)	The solution is stirred before the measurement. Pause will be allowed to elapse before the measurement.
(Switch on stirrer)	The stirrer will be switched on if Stir solution during measurement is activated.
Measure standard	The potential of the standard is measured.
(Switch off stirrer)	The stirrer will be switched off if the measured value has been accepted and if Stir solution during measurement is activated.
Calculate calibration data	The cell constant is calculated, the limits checked and, if necessary, an appropriate message displayed. The calibration data will be added to the sensor data for the particular sensor.

Optional steps are shown in brackets.

4.9 Electrode test for pH electrodes (ELT)

For pH electrodes you can carry out an automatic electrode test which allows the quality of the electrode used to be evaluated. As the result you will obtain various information about the characteristic measuring properties of your pH electrode (slope, response time etc.). The concluding evaluation of the electrode is carried out by checking the results obtained against preset limit values. If the electrode test has been finished successfully then the calibration data is stored together with the sensor data of the used sensor.

These limit values are stored in the software for the three most frequently used types of Metrohm pH electrodes: **standard electrodes**, **gel electrodes** and **non-aqueous electrodes**. You can also define your own limits (see *Section 3.14.8*). The specific classification of the electrode system is defined by the reference system used. You find an overview for these electrode types and the corresponding limit values on *page 268*.

Faulty electrodes frequently show certain combinations of measured results of the electrode test which lie outside the preset limits. This permits more detailed information to be given about possible causes and recommended measures.

Buffers

You need faultless pH 4, pH 7 and pH 9 buffers for carrying out the electrode test. We recommend the use of suitable Metrohm buffers. In principle the electrode test can also be carried out with any of the stored sets of buffers.

The buffers must be measured in the following order:

1. pH 9
2. pH 4
3. pH 7



Note!

Particularly with buffer pH 9 you should make certain that it is in a faultless condition. By absorption of CO₂ from the ambient air this buffer can easily vary from its specified pH value and therefore produce incorrect test results.

Stirrer

A stirrer must be connected for the electrode test.

Temperature

Please ensure that the whole electrode test is carried out at a constant temperature. As the temperature has a great influence on the response time you should work at room temperature if possible. The preset limit values are set for 25 °C.

Electrode test param.

Under **Electrode test parameters** you can edit the parameters for the electrode test sequence.

- **Buffer type:** Selects a predefined buffer series for the calibration. The following buffer series are available: **Metrohm, NIST, DIN, Fluka Basel, Mettler, Merck Titrisol, Radiometer, Merck CertiPUR, Baker, Hamilton, Precisa**. The temperature tables for the buffer series can be found in *Section 6.4*.
- **Sample Processor:** If the calibration is carried out with a Sample Processor then the buffers are changed automatically. That is why there is no request of the calibration temperature at the start of the calibration. The value entered below is used.

For calibrations with a Sample Processor connected via a remote box the parameter **Remote** must be activated. When the measurement of a buffer has been completed the Titrando sends a signal to the Sample Processor via the remote connection (EOD, see *Section 6.2.2*). The Sample Processor then switches to the next buffer.

For automatic calibrations with the USB Sample Processor the parameter **USB** must be selected. The CAL command must be called up in a subsequence (see *Section 4.12.6*) with the subsequence option "**Cycles = Calibration**". In order to change the calibration solution a MOVE command (see *Section 4.12.1*) must be inserted before the CAL command with the target "**Calibration pos.**". The 1st calibration position must be defined in the rack table (see *Section 3.10.5*) as a sample position or as special beaker. If a sample position has been given as the 1st calibration position then it is essential that the other calibration solutions are placed in the directly following rack positions. If special beakers are used for the calibration then there must be as many special beakers defined as buffers or standard solutions are required for the calibration. The special beakers do not need to be placed in rack positions that directly follow each other.

- **Electrode type:** Select the electrode type.
 - Standard:** Electrodes containing, e.g., KCl solution as reference electrolyte.
 - Gel:** Electrodes containing Idrolyte as reference electrolyte.
 - Non-aqueous:** Electrodes containing a non-aqueous reference electrolyte, e.g. TEABr in ethylene glycol or LiCl in ethanol.
 - Custom:** Under **System/Templates** you can define your own electrode type.
- **Temperature:** Manually entered calibration temperature. If a temperature sensor is connected and temperature measurement is set to **automatic** or **continuous** under **Sensor** (see *Section 4.1.5*) then the temperature will be measured. If **off** is defined then the temperature is requested after the start (except the calibration is carried out with a Sample Processor).

The parameters for **Control device, Sensor** and **Stirrer** are described in *Section 4.1.5*.



Note!

Make sure that the sensor to be calibrated has been selected under **Edit command/Sensor**. This is the only way to ensure that the **calibration data** for this sensor is stored in the correct place under **System/Sensors**.

Sequence of the electrode test



Note!

In order to obtain realistic response times the electrode should be immersed in each buffer at about the same time as the measurement is started and it should be positioned directly above the stirrer which has already been switched on.

Start the calibration command	
Measure or enter the calibration temperature	If a temperature sensor is connected then the temperature will be measured. Otherwise a query will appear and the temperature must be entered manually.
Immerse electrode into buffer pH 9	Confirm the displayed message with [OK] .
Measure buffer pH 9	The stirrer is switched on. The potential of buffer pH 9 is measured; at first 3 min with stirring, then 1 min without stirring.
Immerse electrode into buffer pH 4	Confirm the displayed message with [OK] .
Measure buffer pH 4	The stirrer is switched on. The potential of buffer pH 4 is measured; at first 3 min with stirring, then 1 min without stirring.
Immerse electrode into buffer pH 7	Confirm the displayed message with [OK] .
Measure buffer pH 7	The stirrer is switched on. The potential of buffer pH 7 is measured; at first 3 min with stirring, then 1 min without stirring.
Calculate calibration data	The rating of the electrode is ascertained. The calibration data will be added to the sensor data for the particular sensor.

Limit values of the three electrode types

	Rating		
	<i>Excellent electrode</i>	<i>Good electrode</i>	<i>Usable electrode</i>
Electrode type "Standard"			
Streaming potential	2.5 mV	3.0 mV	4.0 mV
Drift	2.0 mV/s	2.5 mV/s	3.0 mV/s
Slope min.	96.5 %	96.0 %	95.0 %
Slope max.	101.0 %	102.0 %	103.0 %
Response time	45 s	50 s	60 s
Lower limit U _{off}	-15 mV		
Upper limit U _{off}	15 mV		
Electrode type "Gel"			
Streaming potential	3.0 mV	3.5 mV	4.5 mV
Drift	2.5 mV/s	3.0 mV/s	4.0 mV/s
Slope min.	96.5 %	96.0 %	95.0 %
Slope max.	101.0 %	102.0 %	103.0 %
Response time	60 s	75 s	90 s
Lower limit U _{off}	-15 mV		
Upper limit U _{off}	15 mV		
Electrode type "Non-aqueous"			
Streaming potential	3.0 mV	4.5 mV	6.0 mV
Drift	5.0 mV/s	7.0 mV/s	9.0 mV/s
Slope min.	88.0 %	80.0 %	70.0 %
Slope max.	120.0 %	130.0 %	140.0 %
Response time	60 s	75 s	90 s
Lower limit U _{off}	-10 mV		
Upper limit U _{off}	70 mV		

Possible errors of the electrode test

<i>Test criterion</i>	<i>Message</i>	<i>Measure</i>
pH 9: The drift in stirred solution is > 1 mV.	General problem	<ul style="list-style-type: none"> - Connect electrode. - Replace defective electrode cable. - Clean diaphragm (see electrode leaflet). - Replace electrode.
pH 9: -10 mV < U(unstirred) < 10 mV and the sum of drift values after 1, 2, 3 und 4 min is < 12 mV/min.	Short circuit	Replace electrode.
A response time does not meet the limit value for the rating "Usable electrode".	Glass membrane / Diaphragm	Clean diaphragm (see electrode leaflet).
The pH values are not defined for all the buffers at the measured temperature.	No buffer data	Repeat electrode test at a temperature at which the pH values of all the buffers are defined.
All the slopes meet the limit values for the rating "Usable electrode" and U _{off} is outside the given limits.	Unsuitable reference electrode	<ul style="list-style-type: none"> - Repeat electrode test with suitable reference system. - Replace contaminated reference electrolyte. - Select electrode type = Custom and adjust limits for U_{off}.
The streaming potential is too high.	Contaminated diaphragm	Clean diaphragm (see electrode leaflet).
Two slopes do not meet the limit values for the rating "Usable electrode".	Wrong buffer	Repeat electrode test with buffers pH 4, 7 und 9.
All the slopes do not meet the limit values for the rating "Usable electrode".	Partial short circuit	Check temperature sensor or enter correct calibration temperature.

4.10 Dosing and liquid handling

With the dosing commands you can add a fixed volume in the method sequence; exchange or dosing units can also be prepared and emptied automatically. Complex dosing tasks can be carried out comfortably with the liquid handling commands.

4.10.1 Dosing (ADD)

The ADD command is used to add a preset volume of a solution.

Dosing parameters

- **Volume** (d): Volume to be added.
- **Dosing rate** (d): Rate at which the volume is to be added. The maximum dosing rate depends on the cylinder volume of the exchange or dosing unit used (see *Section 3.8.6*).
- **Filling rate** (d): Rate at which the dosing cylinder is refilled after addition has been carried out. The maximum filling rate depends on the cylinder volume of the exchange or dosing unit used (see *Section 3.8.6*).

Control device

Under **Control device** you can select the control device (Titrande, USB Sample Processor etc.) with which the dosing or liquid handling command is to be carried out. This button will only be shown when several control devices have been configured under **System/Device manager** (see *Section 3.10*). The device names are always shown in the selection list.

The parameters for **dosing devices** and **stirrers** are described in *Section 4.1.5*. Selection of the **direct parameters** is described in *Section 4.1.6*.

4.10.2 Liquid handling (LQH)

This command can be used to carry out liquid handling tasks with a Dosino (type 700 or 800) dosing device. Together with a USB Sample Processor the versatile possibilities of the Dosino can be used to the full extent. The four ports of the dosing units for the Dosino can be used as inlet or outlet ports as defined by the user. This means that not only simple dosing and filling processes are possible, but complex liquid handling tasks such as pipetting and sample transfer can be carried out without any problems. This requires several LQH and automation commands that are best grouped together in subsequences (see *Section 4.12.6*).

The dosing functions are to be used in such a way that, in addition to the function, the port at which the function is to be carried out is also given. This means the dosing unit inlet or outlet to which the valve disk first moves in order that the required function is carried out. The definitions of the ports is described in *Section 6.5.1*.

Liquid handling param.

- **Function:** Selects the possible working steps.
 With **Dosing** the given volume is added. Automatic filling takes place neither before nor after the command.
Fill the cylinder can take place from a freely selectable port. The valve disk then remains at the selected port.
 With **Aspirate** liquid is aspirated via the given port. As with Dosing, the cylinder is not automatically filled either before or after the command. It should be possible for the aspirated volume to be removed with a single piston stroke.
 With the **Eject** function the whole cylinder content is ejected via the given port. In contrast to the function "End volume" the piston is pressed down to the stop, i.e. past the maximum volume mark. This command should only be used for preparing the dosing unit before the pipetting sequence.
 With the command **Exchange position** the cylinder is filled via the given port. This means that, for example, air can be aspirated via Port 4. The valve disk is then rotated to Port 2 and the dosing drive can be removed from the dosing unit.
 With **Change port** the valve disk is only moved to the given port; no piston movement takes place.
 As the dosing units are exchangeable, the coupling of the Dosino piston rod (spindle) has a slight mechanical tolerance that can be noticed when the piston changes its direction of movement. This tolerance can be compensated with the command **Compensate**. A short piston movement is first made in the same direction as the previous movement; this is followed by a piston movement in the reverse direction.
 The whole cylinder content is ejected via the selected port with **End volume**. The piston is lowered to the maximum volume mark i.e. until 10'000 pulses have been dosed. This command should be used for pipetting functions to empty the cylinder.
- **In-/Outlet:** Selects the port, with which the liquid handling command should be carried out.
- **Volume:** Here you enter the volume to be processed.
- **Rate:** Rate at which the commands **Dosing, Fill, Aspirate, Eject, Exchange position** and **End volume** are carried out. Aspirating and ejecting the sample should be done with a rate < 10 mL/min.

The item **Control device** is mentioned in *Section 4.10.1*, the parameters for the **Dosing device** are described in *Section 4.1.5*.

A schematic command sequence is explained in *Section 6.5.3*.

4.10.3 Preparing (PREP) and emptying (EMPTY)

Preparation is used to rinse the cylinder and the tubing. **Empty** is used to empty the cylinder and the tubing. The empty command is only available for **Dosino**-type dosing devices.

- **Control device:** Selects the control device (Titrande, USB Sample Processor etc.) to which the dosing device is connected and which is to be prepared or emptied. This button is only shown when several control devices have been configured under **System/Device manager** (see *Section 3.10*). The device names are always shown in the selection list.
- **Dosing device:** Dosing device to be prepared or emptied. All dosing device connections (MSB) are always shown.
- **Titration:** Titration with which the preparation or empty command is to be carried out. The titration can be selected from the list of titrations which have been defined under **System/Titrations**. If intelligent exchange or dosing units are used then a check will be made in the method sequence that the correct titration is present in the connected dosing device and whether the type of dosing device is correct. With non-intelligent exchange or dosing units the cylinder volume is checked. At the start of the command the validity of the titer and the expiry date of the selected titration will be checked as well as the GLP test interval for the exchange or dosing unit. The tubing parameters defined under **System/Titrations** for the selected titration will be used for preparing and emptying the exchange or dosing unit. The parameters for the preparation are also defined under **System/Titrations**. If no titration has been defined then the standard tubing parameters and the default parameters for the preparation will be used (see *Section 3.8.6*).
- **Cylinder volume to** (PREP only): Select the port of the Dosino where the titration is ejected. This parameter is only active when the titration is not defined. If a titration has been defined, the cylinder volume is ejected via the port defined as dosing port for preparing/emptying (see *Section 3.8.6*).
- **Air inlet** (EMPTY only): Select the port where the air is aspirated. This parameter is only active when the titration is not defined. If a titration has been defined, the port defined as special port is used (see *Section 3.8.6*).

A detailed description of the preparation and emptying sequences is given in *Section 3.24.2, p. 182 and p. 183*.

4.10.4 Monitored dosing (DOS)

A predefined volume of a solution is dosed with the DOS command. The measured value and the temperature are monitored simultaneously.

Dosing parameters

- **Dosing criterion:** Two parameters from the following can be defined: **Volume**, **Dosing rate** and **Dosing time**. The third parameter is calculated according to the following formula:

$$\text{Volume} = \text{Dosing time} \cdot \text{Dosing rate}$$

If continuous dosing is required, a tandem dosing setup (see Section 4.1.5) can be used i.e. dosing is carried out with a combination of two dosing devices. The second dosing device is dosing while the first one is being filled and vice versa.

Depending on the type of task one of the following types of dosing can be used:

Volume / Dosing rate – You define the volume to be dosed and the desired dosing rate. The filling times lengthen the dosing process.

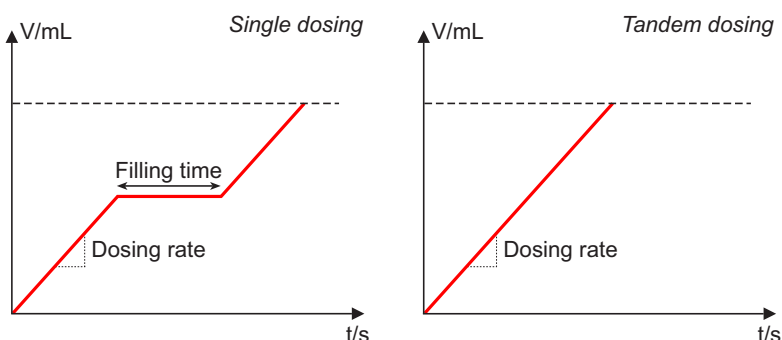


Fig. 4.18: Definition of volume and dosing rate

Volume / Dosing time – You define the volume and the time in which this volume is to be dosed (particularly suitable for synthesis applications). The dosing rate is automatically optimized by the Titrando (see formula above).



Attention!

The time defined as **Dosing time** corresponds to the net dosing time t_1+t_2 , i.e. the filling time of the exchange or dosing unit is not taken into account.

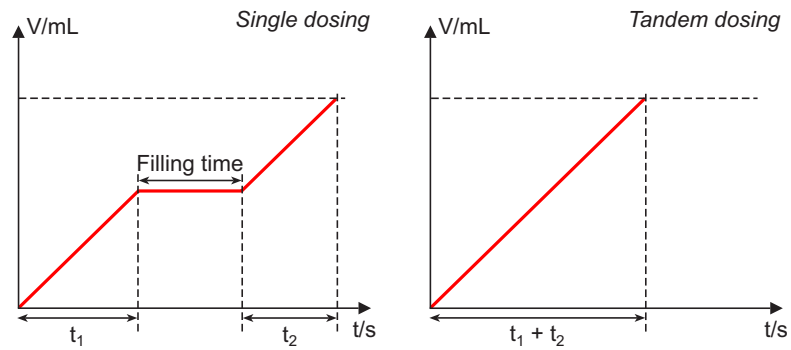


Fig. 4.19: Definition of volume and dosing time

If the dosing rate resulting from the settings cannot be achieved dosing is carried out at maximum rate.

The following formula can be used to estimate whether the maximum dosing rate is necessary or not:

$$\text{Dosing rate} = \text{Desired flow rate in mL/min} \cdot 2.22$$



Note!

This formula applies only for using a single dosing device. The dosing rate is equal to the flow rate for tandem dosing.

If the required dosing rate exceeds the maximum dosing rate for the selected exchange or dosing unit (or cylinder volume, see Section 3.8.6), then a larger cylinder volume must be selected.

Dosing rate / Dosing time – You define the dosing rate and the time in which dosing is to be carried out. As in the previous case, the filling times are not taken into account.

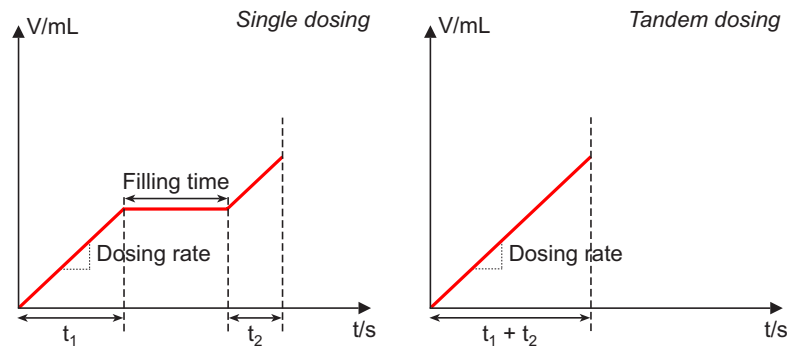


Fig. 4.20: Definition of dosing rate and dosing time

Flow rate of a single dosing device

The cylinder volume and the filling time of the exchange or dosing unit must be taken into account for the calculation of the effective flow rate.

Max. flow rates for different cylinder volumes:

<i>Cylinder volume</i>	<i>Max. flow rate</i>	
	<i>Exchange unit</i>	<i>Dosing unit</i>
1 mL	approx. 80 mL/h	---
2 mL	---	approx. 170 mL/h
5 mL	approx. 400 mL/h	approx. 430 mL/h
10 mL	approx. 800 mL/h	approx. 860 mL/h
20 mL	approx. 1.6 L/h	approx. 1.7 L/h
50 mL	approx. 4 L/h	approx. 4.3 L/h

Filling times

Filling times are not included in the calculation of the dosing rate by the Titrand. The filling times (including valve switching) can be estimated according to the following formula:

$$\text{Filling time in s} = \frac{\text{Maximum filling rate}}{\text{Actual filling rate}} \cdot t + 4\text{s}$$

t = 20 s (for exchange units)
18 s (for dosing units)

The maximum filling rate depends on the cylinder volume of the exchange or dosing unit used (see *Section 3.8.6*). In the table below the approximate filling times (including valve switching) are given for various cylinder volumes (exchange and dosing unit) at different filling rates:

<i>Cylinder volume</i>	<i>Filling time in s</i>			
	<i>maximum</i>	<i>100 mL/min</i>	<i>50 mL/min</i>	<i>10 mL/min</i>
1 mL	24 / ---	---	---	---
2 mL	--- / 22	---	---	---
5 mL	24 / 22	---	---	34
10 mL	24 / 22	---	---	64
20 mL	24 / 22	---	28	124
50 mL	24 / 22	34	64	304

Example:

1 L reagent has to be dosed within 1 hour with a 50 mL exchange unit. What is the dosing rate?

Total duration = 60 min
 Volume = 1000 mL
 Filling time = 24 s (at max. filling rate)
 Cylinder volume = 50 mL

$$\text{Number of refills} = \frac{\text{Volume}}{\text{Cylinder volume}} = \frac{1000}{50} = 20$$

If the division delivers an integer number, the last filling is no longer a refilling and must be deducted. In our example, 19 refills are necessary. There is no dosing during this time i.e. the net dosing time is $3600 \text{ s} - 19 \cdot 24 \text{ s} = 3144 \text{ s} = 52.4 \text{ min}$

The dosing rate is thus

$$1000 \text{ mL} / 52.4 \text{ min} = 19.1 \text{ mL/min}$$

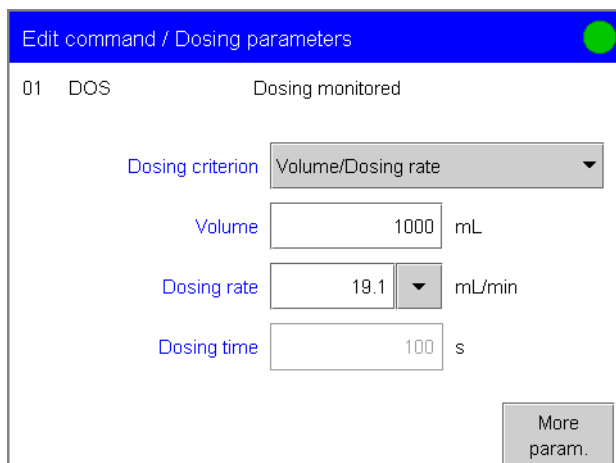
Summary in a formula:

Dosing rate in mL/min:

$$= \frac{\text{Volume}}{\text{Total duration} - \text{No. of refills} \cdot \text{Filling time} \cdot 1/60}$$

$$= \frac{1000}{60 - 19 \cdot 24 \cdot 1/60} = 19.1$$

Parameterization:



- **Volume:** Volume to be added.
- **Dosing rate:** Rate at which the volume is added. The maximum dosing rate depends on the cylinder volume of the exchange or dosing unit used (see *Section 3.8.6*).
- **Dosing time:** Time while the reagent is being dosed i.e. the filling time is not taken into account.
- **Temperature:** Manually entered dosing temperature. If a temperature sensor is connected and temperature measurement is set to **automatic** or **continuous** under **Sensor** (see *Section 4.1.5*) then the

temperature will be measured continuously. The value is used for temperature compensation in pH measurements.

- **Time interval MP:** Time interval for entering a measuring point in the list of measuring points. The list of measuring points can contain max. 1000 measuring points.
- **Pause:** Waiting time, e. g. for electrode equilibration, after the start of the method.

Stop conditions

The conditions for terminating the dosing are defined under **Stop conditions:**

- **Stop volume:** Stops when the preset volume has been added since the start of the dosing. You should adapt the stop volume to suit the size of your vessel in order to prevent it from overflowing.
- **Stop time:** Stops when the preset time has elapsed after the start of the dosing.

If several stop conditions have been set then the first criterion to be fulfilled will stop the dosing.

- **Filling rate:** Rate at which the dosing cylinder is refilled after the dosing. The maximum filling rate depends on the cylinder volume of the exchange or dosing unit used (see *Section 3.8.6*).

Monitoring

The parameters for monitoring the **measured value** as well as the **temperature** are defined under **Monitoring**. Remote signals or RS commands can be assigned to the monitored quantities. This can be used, for example, to switch a thermostat on/off if necessary.

- **Measured quantity:** Select the measured quantity being monitored.

The remaining parameters are described in the section about the STAT titration (see *Section 4.1.4*).

The item **Control device** is mentioned in *Section 4.10.1*, the parameters for the **Sensor**, **Dosing device** and **Stirrer** are described in *Section 4.1.5*.

4.11 Communication

With the communication commands SCAN and CTRL you can scan and set remote lines at a connected remote box. The connection of the remote box is described in the Installation Instructions for the Titrandu. The pin occupancy of the remote connection and the functions of the individual remote lines are described in *Section 6.2*.

The commands SCAN RS and CONTROL RS are for the communication with peripheral devices which are connected via a serial RS-232 interface.

4.11.1 Scanning lines (SCAN)

Definition of input signals which are to be waited for before the next command is carried out (SCAN).

- **Control device:** Selects the control device (Titrandu, USB Sample Processor etc.) to which the remote box is connected. This button is only shown when several control devices have been configured under **System/Device manager** (see *Section 3.10*). The device name is always shown in the selection list.
- **Remote box:** Remote box at which the lines are to be scanned. All the remote box connections (MSB) will always be shown.
- **Input signal:** Selects the signal from the templates which have been defined under **System/Templates/Input lines** or enters the binary pattern directly. Please consult the **online help** for the input of the binary pattern.
- **Timeout:** You can define a time after which an action should be carried out in case the signal pattern has not been recognized.
- **Timeout action:** The action defined here will be carried out if the time interval has expired.

Input lines that are of no interest or for which no defined condition can be predicted should be masked with an asterisk (*).

The templates are described in *Section 3.14.4*.

4.11.2 Setting lines (CTRL)

Definition of output signals which are to be transmitted (CTRL).

- **Control device:** Selects the control device (Titrandu, USB Sample Processor etc.) to which the remote box is connected. This button is only shown when several control devices have been configured under **System/Device manager** (see *Section 3.10*). The device name is always shown in the selection list.
- **Remote box:** Remote box at which the lines are to be set. All the remote box connections (MSB) will always be shown.
- **Output signal:** Selects the signal from the templates which have been defined under **System/Templates/Output lines** or enters the binary pattern directly. Please consult the **online help** for the input of the binary pattern. The pulse length for **p** is fixed at 200 ms. If you

wish to use a pulse with a pulse length other than 200 ms then you must define a corresponding template.

We recommend that non-relevant output lines are also masked with an asterisk (*) in order that the condition of these lines is not altered.

The templates are described in *Section 3.14.5*.

4.11.3 Receive data (SCAN RS)

Definition of the parameters for receiving data via a serial RS-232 interface.

- **Serial port:** Selection of the RS-232 interface which the peripheral device is connected to.
- **Data string:** Enter the desired data string here. "*" can be used for one or more characters.
- **Timeout:** You can define a time after which an action should be carried out in case the signal pattern has not been recognized.
- **Timeout action:** The action defined here will be carried out if the time interval has expired.

4.11.4 Send data (CONTROL RS)

Definition of the parameters for sending data via a serial RS-232 interface.

- **Serial port:** Selection of the RS-232 interface which the peripheral device is connected to.
- **Data string:** Enter the desired data string here. All characters according to ASCII code can be used. Please consult the **online help** for how to enter the data string.

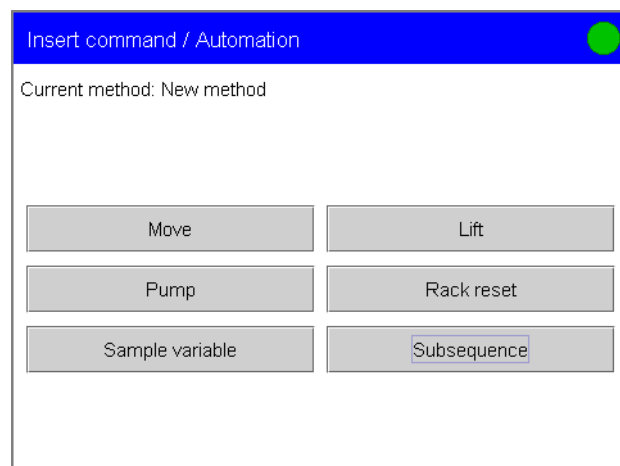


Note!

Each command is terminated automatically with carriage return + line feed.

4.12 Automation

The automation commands, with the exception of the subsequence, are only active when a USB Sample Processor has been configured in the Device manager (see *Section 3.10*). A connected USB Sample Processor is controlled with these commands in the method sequence.



4.12.1 Move (MOVE)

The MOVE command is used to move to a rack position or an external position.

- **Tower:** The required tower can be selected here. Both Tower 1 and Tower 2 are always available for selection, even if your USB Sample Processor only has one tower. If you accidentally select the non-existent tower then the corresponding error message will appear after the start of the method.
- **Destination:** This is the target position for the MOVE command.
 - Sample** gives the rack position that is defined by the current sample variable. The sample variable is automatically increased by one after each method sequence. Under **Method options/Start options** you can switch off this automatic increase. With the SAMPLE command (see *Section 4.12.5*) the sample variable can also be selectively altered.

If the USB Sample Processor is equipped with a Swing Head then four **external positions** can be moved to.

Special beakers must be defined in the rack table under **Edit device/Rack tables**.

When selecting **Rack position** each absolute position of a rack can be moved to directly.

With **Current sample +/-** a particular rack position relative to the current sample as defined by the sample variable can be moved to.

With **Next/Previous position** the next or previous rack position will be moved to starting from the current rack position.

Calibration pos. is used when automatic calibration is to be carried out with a USB Sample Processor (see *Section 4.7*).

The sample rack can be rotated by a certain increment independently from a rack position with the function **+/- rotate**.

The robotic arm can also be swung by a certain increment independently from the position with **+/- swing**.

The values of the rotation and swing increment are defined in the device properties of the tower and of the Swing Head respectively (see *Section 3.10.5*).

- **Beaker test action:** If no sample is present at the rack position that has been moved to then the action selected here will be carried out, provided that the beaker sensor has been activated in the rack table (see *Section 3.10.5*).
- **Options:** The **shift rate** and the **shift direction** can be edited here. The **swing rate** defines the rate of the robotic arm when moving to a rack position, a special beaker or an external position.

4.12.2 Lift (LIFT)

The lift can only be moved when the USB Sample Processor is at a valid rack position. In manual control "--" indicates that the lift is at an invalid position. This is the case, for example, after a manual rack reset (see *Section 3.24.6*).

- **Tower:** The selected lift position is moved to by the selected tower. Both Tower 1 and Tower 2 are always available for selection, even if your USB Sample Processor only has one tower.
- **Lift position:** In addition to any lift position in mm the freely definable positions Work position, Shift position, Rinse position and Special position can be selected. These settings apply for sample positions, each special beaker and the external positions. The lift positions are defined in the rack table in the Device manager of the USB Sample Processor (see *Section 3.10.5*). However, they can also be assigned directly in the manual control of the USB Sample Processor (see *Section 3.24.6*). A lift height of 0 mm corresponds to the "Home position", i.e. the lift is being located at the upper stop position. Please ensure that no lift position exceeds the maximum stroke path defined in the device properties of the tower.
- **Lift rate:** The rate at which the lift is moved can be edited here.

4.12.3 Pump (PUMP)

The PUMP command is used to control the pumps mounted on or connected to the tower of the USB Sample Processor.

- **Tower:** This is the tower at which the selected pump is to be switched. Both Tower 1 and Tower 2 are always available for selection, even if your USB Sample Processor only has one tower.
- **Pump:** Selects the pump that is to be switched. With "1+2" both pumps will be switched at the same time.
- **Status/Duration:** A pump can be switched on or off, or switched on for a certain time.

4.12.4 Rack reset (RACK)

With the command **Rack reset** the rack, lift and robotic arm are reset, the rack code is read off and the corresponding rack data is transferred to the USB Sample Processor. At the same time the sample variable is reset to one.

- **Check rack:** The rack which is put on can be checked at the start of the method. In this way you can ensure that the method can only be carried out with this rack. This means that you have to select the desired rack in the start options under **Check rack**.

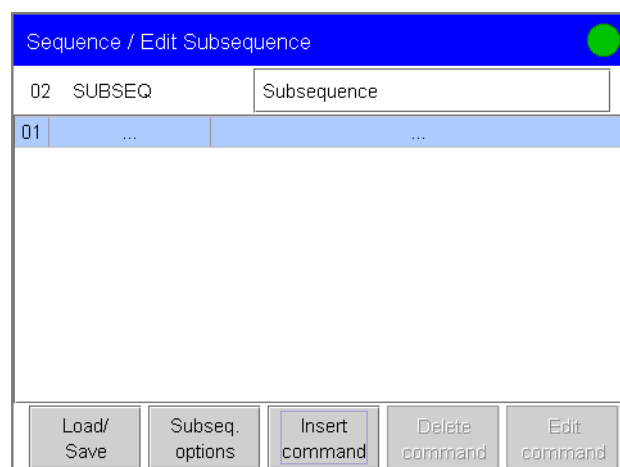
4.12.5 Sample variable (SAMPLE)

The sample variable describes the current position of the sample at the USB Sample Processor. At the end of a method sequence it is automatically increased by one. It is again reset to one at the start of the system and after a Rack reset. With the SAMPLE command the sample variable can also be selectively altered. For example, a SAMPLE command can be inserted in order to prevent the automatic increase at the end of a method. This automatic increase can also be switched off under **Method options/Start options** (see *Section 3.16.7*).

- **Sample variable:** The sample variable can be set to a particular value with "=" or, based on the current value, altered with "+" or "-".
- **Value:** This is the amount by which the sample variable is to be altered.

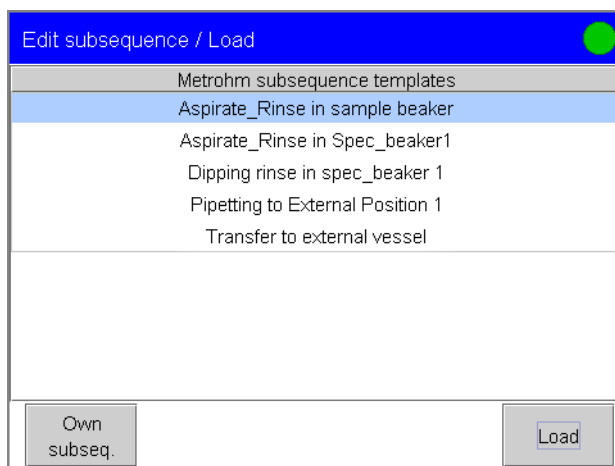
4.12.6 Subsequence (SUBSEQ)

With more complex tasks in particular, such as rinsing procedures or liquid handling (see *Section 4.8*), it is advisable to group command sequences together to form a subsequence. Subsequences are managed in the same way as method commands. A maximum of 99 commands can be grouped together to form a subsequence. There is no limitation on the number of subsequences contained in a method.



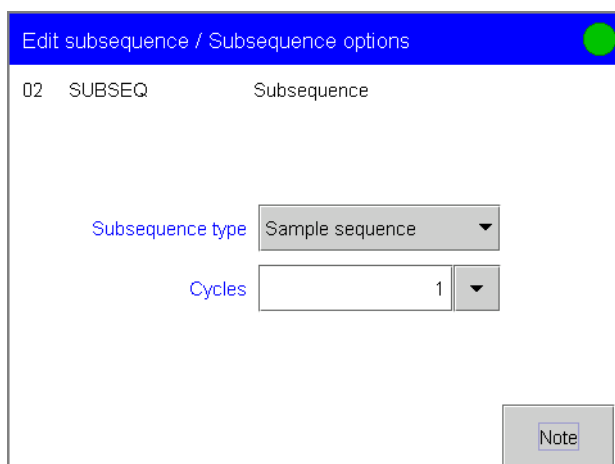
[Load/Save] is used to load stored subsequences or to save new subsequences. This means that they are available for all methods and only have to be drawn up once.

The list with templates for subsequences is displayed under **Edit Sub-sequence/Load**:



Open the list with your **[Own subsequences]**. You have now the possibility to load or to delete your own subsequence.

Under **[Subsequence options]** parameters are set that refer to the whole subsequence:



- Subsequence type:** The type of subsequence is entered here. A **Sample sequence** is carried out each time that a method is run. The **Start sequence** is only carried out at the start of a sample series when the autostart counter = 1. If a subsequence is only to be carried out for the last sample in a series, i.e. when the autostart counter has reached its set value, then it is defined as the **End sequence**. The **Stop sequence** will only be carried out when a method is terminated because of the following cases:

 - Manual termination with the **[STOP]** fixed key
 - Termination because of an error
 - Termination by remote signal via the Control remote box

If the method is ended regularly then the stop sequence is not carried out. The sample sequence can be used in this case.

The **Conditioning sequence** will be carried out just before the conditioning. It gives you the opportunity, for example, to start a connected Polytron® high-frequency homogenizer and to set its stirring rate before the start of the conditioning. Use the CONTROL RS command for this.

- **Cycles:** A subsequence is repeated in accordance with the number of runs. "**Calibration**" is required if automatic calibration is to be carried out with a USB Sample Processor. Apart from the CAL command, the subsequence contains a MOVE command to move to the calibration solutions. It is processed until the number of buffers or standards defined in the calibration command has been reached.

Note

In a **[Note]** a short text can be used to describe e. g. what the subsequence is used for.

With **[Insert command]** you can insert a command in front of the selected line.



Note!

In contrast to general method programming, the choice of commands is limited. With the exception of calibration, no commands for recording or evaluating measured values (e. g. titration, measurement) can be inserted in a subsequence. Only one CAL command can be inserted in a subsequence.

[Delete command] removes the selected command from the list. The parameters for the selected command can be edited with **[Edit command]**.

4.13 Various commands

Various commands are brought together in the command group **Miscellaneous**: switching the stirrer on/off, defining a waiting period or stopping the run, requesting sample data or common variables, acoustic signal, signing the determination and stopping the method sequence.

4.13.1 Stirring (STIR)

The STIR command is used to switch a connected stirrer on or off.

- **Control device**: Selects the control device (Titrande, USB Sample Processor etc.) to which the stirrer which is to be controlled is connected. This button is only shown when several control devices have been configured under **System/Device manager** (see *Section 3.10*). The device name is always shown in the selection list.
- **Stirrer**: Selects the stirrer. All the stirrer connections (MSB) will always be shown.
- **Status/Duration**: The stirrer can be switched on or off, or switched on for a certain time. When the stirrer is switched on, you can set the stirring rate.
- **Stirring rate**: You can test the optimal stirring rate manually (see *Section 3.24.3*). The stirring direction changes as the sign changes. The default setting **8** corresponds to 1000 rpm (see *Section 4.1.5*, *Fig. 4.14*).

4.13.2 Waiting (WAIT)

This command can be used to pause the method sequence.

- **Hold sequence**: When this function is activated the method sequence will be halted (HOLD) until it is continued manually with **[Continue]**.
- **Waiting time**: If **Hold sequence** is deactivated then a waiting time can be entered. The method sequence will restart automatically when this waiting time has elapsed.
- **Message**: When this function is activated the text for the message will be shown during the waiting time.
- **Message text**: Text to be shown during the waiting time.

4.13.3 Requesting sample data and common variables (REQUEST)

With the REQUEST command you can request sample data (sample identification 1, sample identification 2 and sample size) or a common variable during the method sequence. You can choose whether the run is to be stopped or whether it should continue in the background.

- **Sample identification:** Select the sample identification(s) to be requested in the sequence.
- **Sample size:** If this function is active then the value for the sample size will be requested.
- **Sample size unit:** If this function is active then the unit for the sample size will be requested.
- **Common variable:** Selects the common variables to be requested in the sequence.
- **Hold sequence:** If this function is switched on then the sequence will be halted for the request. If it is switched off then the method will continue to run in the background until the following titration, measurement or calibration has been completed.

4.13.4 Acoustic signal (BEEP)

The BEEP command is used to produce an acoustic signal during the method sequence.

- **Number of sounds:** Number of tones for the signal in the method sequence. For PC Control the tone selected in the Control panel under **Sounds and Audio Devices** will be used. With Touch Control the number of sounds cannot be altered.

4.13.5 Signature (SIGN)

The SIGN command can be used for signing a determination at the end of a method sequence. It must always be inserted at the end directly before the REPORT command, or at the end of the method sequence if a PC/LIMS report is to be transmitted automatically. The method sequence is automatically stopped as soon as the SIGN command is reached. At the same time a switch is made to the result display. The method will only be continued when the method has been signed. The parameters for signing determinations are described in Section 3.7.5 and 3.7.7.

4.13.6 End (END)

The method sequence will stop as soon as the command END is reached. This is a good idea if you only want to test the first part of a method. The END command has no parameters that can be edited.

5 Troubleshooting – Maintenance

This section contains troubleshooting information and a description of the diagnosis functions integrated in Touch Control and PC Control. For Touch Control a description is given of how to change the batteries and carry out a "RAM initialization".

5.1 Troubleshooting

This section describes several problems that could occur when operating the system together with possible causes and their remedies.

5.1.1 Editing methods

<i>Problem</i>	<i>Possible cause</i>	<i>Remedy</i>
The required command cannot be inserted with Insert command.	The use of the command has been deactivated under Dialog options/Command list .	Activate the command under Dialog options/Command list (see <i>Section 3.7.3</i>).
An evaluation (EVAL command) cannot be inserted.	A data producing command (titration or measurement) to which the evaluation could be applied is missing.	First insert a titration or measurement command and then the evaluation (see <i>Section 4.3</i>).
An evaluation (EVAL command) is shown in red in the list of commands.	A data producing command (titration or measurement) is missing, or the data producing command has been replaced by another one, (e. g. DET pH by DET U) to which the evaluation cannot be applied.	Delete the EVAL command and first insert the titration or measurement command and then the evaluation (see <i>Section 4.3</i>).

5.1.2 Sample series

<i>Problem</i>	<i>Possible cause</i>	<i>Remedy</i>
The method cannot be entered in the sample data silo.	The use of the sample assignment table is switched on under System/Templates /Sample data . The method assigned to the sample identification will be automatically loaded at the start of the determination.	Switch off the use of the sample assignment table under System/Templates/Sample data (see <i>Section 3.14.2</i>).

5.1.3 Results, calculations and statistics

<i>Problem</i>	<i>Possible cause</i>	<i>Remedy</i>
No statistics are carried out for a result.	The Statistics function has not been activated in the method under Sequence/Method options .	Activate the statistics function under Sequence/Method options (see <i>Section 3.16.4</i>).
	No Variable for mean has been selected in the method for the result calculation.	Select a Variable for mean in the CALC command under Edit result/Result options for the result (see <i>Section 4.4.1</i>).
	The Statistics function is switched off under Control .	Activate the Statistics function under Control (see <i>Section 3.17.1</i>).
Results have been deleted in the statistics, but the variables (e. g. titer or common variable) have not been reassigned.	If the statistics results are subsequently altered then the assignment is not automatic.	Trigger the assignment of the current statistics results with [Recalculate] under Results (see <i>Section 3.18.8</i>).
The result is not shown in the result silo.	The numbering of the results corresponds to the result variables.	Under Results/Result silo/Properties alter the settings for the result silo display so that the required result is shown (see <i>Section 3.22.1</i>).
	The function Save result in result silo has not been switched on for the result.	Activate this function for the required result in the CALC command under Result options/More options (see <i>Section 4.4.1</i>).

5.1.4 SET titrations

<i>Problem</i>	<i>Possible cause</i>	<i>Remedy</i>
Dosing at the end takes too long and the increments are too small.	Max. rate too low.	Increase the min. rate under Control parameters/User-def. parameters.
	Unfavorable Stop criterion.	Try increasing the Stop drift or select a shorter Delay time.
"Overshoot"	The titration is not controlled properly, i.e. individual increments are not added at the end.	<ul style="list-style-type: none"> - Select the Titration rate slow under Control parameters. - Select a larger Dynamics under Control parameters/User-def. parameters. - Reduce the Max. rate under Control parameters/User-def. parameters. - Reduce the Min. rate under Control parameters/User-def. parameters. - Ensure that the solution is better mixed and that the arrangement of electrode and buret tip is optimal (see Installation Instructions for the Titrande).
	Electrode responds too slowly.	Replace the electrode.
Titration time too long.	Unfavorable control parameters.	<ul style="list-style-type: none"> - Select the Titration rate optimal or fast. - Select a smaller Dynamics under User-defined parameters. - Increase the Max. rate under User-defined parameters. - Increase the Min. rate under User-defined parameters.
Results widely scattered.		Reduce the Min. rate under Control parameters/User-def. parameters.
	Electrode responds too slowly.	Replace the electrode.

5.1.5 KF titrations

<i>Problem</i>	<i>Possible cause</i>	<i>Remedy</i>
Dosing at the end takes too long and the increments are too small or the conditioning takes very long, high drift.	Inappropriate solvent, pH value suboptimal (side reactions)	Change the solvent with problematic samples e. g. 2-methoxyethanol for ketones or aldehydes or a mixture of methanol/glacial acetic acid for amines, see technical literature.
	Leaking titration cell	Check the sealings and the septum and replace them if necessary. Replace the desiccant.
	Min. increment too low	Increase the Min. increment under Control parameters/User-def. parameters.
	Unfavorable Stop criterion.	Try increasing the Stop drift or select a shorter Delay time.
"Overshoot"	The increments at the end of the titration are too large.	<ul style="list-style-type: none"> - Reduce the Max. rate under Control parameters/User-def. parameters. The following experiment gives you a clue for the optimum max. rate: Display the drift throughout conditioning and add sample without starting the titration. Select a value below the maximum drift as max. rate. - Optimize the assembly of electrode and buret tip and improve stirring (see Installation Instructions for the Titrand).
Solution becomes too brown at the end of the titration.	The methanol fraction in the solvent is too low.	Replace the solvent.
	The electrode may be covered.	Wipe off the electrode with acetone.
Solution becomes darker with every titration.		Replace the solvent.
	The electrode may be covered.	Wipe off the electrode with acetone.
	The electrode has a short circuit.	Check the Pt wires and switch on the electrode test.

<i>Problem</i>	<i>Possible cause</i>	<i>Remedy</i>
The drift increases with every titration.	Does your sample evolve water extremely sluggishly?	Adjust the method, add solubilizer, work at increased temperature (poss. use KF oven), see technical literature.
	Are acids esterified in your sample?	Change the solution more frequently and increase the buffer capacity of the solvent.
	Does your sample contain ketones or aldehydes?	Use special reagents suitable for ketones and aldehydes.
	The pH value is no more in the optimal range.	Add buffer solution, see technical literature.
The endpoint is reached "too rapidly".		Reduce the Max. rate under Control parameters/User-def. parameters.
The titration times become longer and longer.	The buffer capacity of the solvent can be depleted with two-component reagents.	Change the solution.
		If the drift increases at the same time, see there.

5.1.6 STAT titrations

<i>Problem</i>	<i>Possible cause</i>	<i>Remedy</i>
The control point is not kept constant (The controller oscillates).	The titration is not controlled properly. Rule of thumb for the minimum rate: expected rate of reaction in $\mu\text{L}/\text{min} / 10$	- Reduce the Min. rate under Control parameters/User-def. Parameters, possibly the Max. rate as well. - Increase the Dynamics under Control parameters/User-def. parameters.
	Insufficient stirring.	Increase the stirring rate.
	Improper assembly of electrode and buret tip.	Make sure that the assembly of electrode and buret tip is correct (see Installation Instructions for the Titrand).)
	Tubes are kinked.	Use new tubes.

<i>Problem</i>	<i>Possible cause</i>	<i>Remedy</i>
	Cylinder volume of exchange/dosing unit is too large.	Use an exchange/dosing unit with a smaller cylinder volume (smaller volume increment per pulse).
	Electrode responds to slowly.	Replace the electrode.
Time for reaching the control point is too long.	Unfavorable control parameters .	<ul style="list-style-type: none"> - Select a smaller Dynamics under User-defined parameters. - Increase the Min. rate under User-defined parameters. - Increase the Max. rate under User-defined parameters.

5.1.7 Sensor data

<i>Problem</i>	<i>Possible cause</i>	<i>Remedy</i>
After calibration the calibration data is not stored together with the sensor data.	In the method the correct Sensor has not been selected in the CAL command.	Take care that the sensor to be calibrated has been selected under Edit command/Sensor (see Section 4.1.5).

5.1.8 Print

<i>Problem</i>	<i>Possible cause</i>	<i>Remedy</i>
The [Print] fixed key is inactive.	The [Print] fixed key is deactivated.	Activate the [Print] fixed key under Dialog options/Fixed keys (see Section 3.7.3).
	The system is in the BUSY status, i.e. a determination is running.	Wait until the determination is finished.
PC Control: empty pages are produced when printing out the result silo report or the statistics overview.	Landscape format has been selected under orientation in the Windows-specific printer settings .	in the Windows-specific printer settings select portrait format as the printout is automatically made in landscape format.

<i>Problem</i>	<i>Possible cause</i>	<i>Remedy</i>
Touch Control: The error message "No printer" is displayed when printing manually or when starting a method with a REPORT command.	The USB printer has been switched off while the Touch Control was running.	Switch on the printer again and switch off and back on the Touch Control.

5.1.9 Manual Operation

<i>Problem</i>	<i>Possible cause</i>	<i>Remedy</i>
The [Manual] fixed key is inactive.	The [Manual] fixed key is deactivated.	Activate the [Manual] fixed key under Dialog options/Fixed keys (see Section 3.7.3).
Manual operation buttons are inactive.	The corresponding hardware is either not connected or not properly connected.	Connect the hardware correctly (see Installation Instructions for the Titrand).
	The appropriate hardware has not been recognized correctly.	Switch off the system and then switch it on again.
	The corresponding hardware is occupied with a determination run.	Wait until the determination is finished.

5.1.10 USB Sample Processor

<i>Problem</i>	<i>Possible cause</i>	<i>Remedy</i>
No Rack Reset can be carried out	The robotic arm can not rotate.	Check the setup settings of the robotic arm in the device manager under Sample Processor/Swing Head/Robotic arm (see Section 3.10.5)

5.1.11 File manager

<i>Problem</i>	<i>Possible cause</i>	<i>Remedy</i>
Files, e. g. methods, which have been saved on a data card by a PC, cannot be read by Touch Control.	Windows Explorer has been used for copying and the correct folder structure has not been maintained (see <i>Section 3.11</i>).	Use PC Control to copy the files.

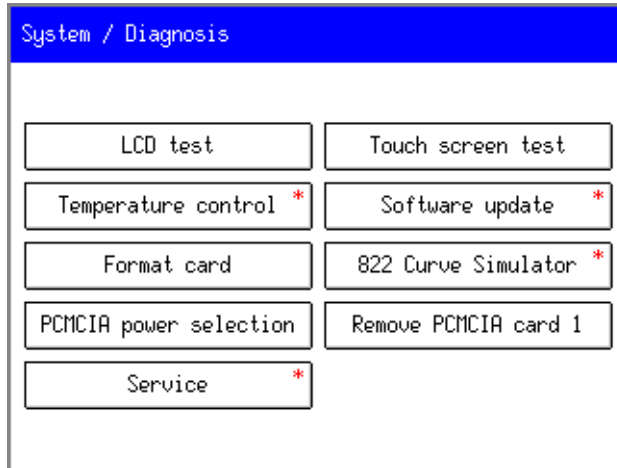
5.1.12 Miscellaneous

<i>Problem</i>	<i>Possible cause</i>	<i>Remedy</i>
Touch Control cannot be switched on.	Touch Control is connected to an MSB socket of the Titrando.	Connect the Touch Control to the Controller socket (see Installation Instructions for the Titrando).
PC Control does not recognize the Titrando.	The PC is connected to an MSB socket of the Titrando.	Connect the PC to the Controller socket (see Installation Instructions for the Titrando).
	The suitable USB driver has not been found.	Remove the USB plug from the PC and reinsert it. Please note that the PC Control software must be installed before the Titrando is connected to the PC (see Installation Instructions for the Titrando).

5.2 Diagnosis

You can carry out selective tests on the Titrand system or trigger special functions.

☞ Select **Diagnosis** in the **System** menu:



The diagnosis functions are written in English and are all available for the Touch Control. With PC Control the selection is limited to those functions marked with an *.

5.2.1 LCD test

With the LCD test you can check the function of the Touch Control display.

- ☞ Press **[LCD test]**. The whole screen appears in white.
- ☞ Continue with **[START]** to show further colors and patterns. You can use **[Back]** to switch back step by step.
- ☞ Check whether the display has any pixel errors or other irregularities. If this is the case please contact your local Metrohm agency.
- ☞ You can exit the LCD test automatically by switching through to the end with **[START]**. It can also be exited at any time with **[Home]**.

5.2.2 Temperature monitoring (Temperature control)

The operating temperature of the Titrand **Temperature TI** is measured inside the housing.

5.2.3 Formatting a memory card (Format card)

- ☞ Select **[Format card]** in order to format a PCMCIA or CompactFlash memory card inserted in the Touch Control.
- ☞ Select the memory card to be formatted (**Card 1 / Card 2**) and the formatting mode. With **normal** the memory card will be completely cleared; with **quick** only the "main folder" of the card will be overwritten with zero so that the whole capacity is again available.
- ☞ Start formatting with **[Format]** and answer the safety query with **[Yes]**.

**Note!**

*In the mode **normal** the memory cards are formatted with a rate of approximately 4 MB/min.*

5.2.4 PCMCIA specification (PCMCIA power selection)

Two different voltages (3.3 V and 5.0 V) are normal for the power supply of the PCMCIA or CompactFlash cards. These are automatically set on the Touch Control with the option **auto VS1/VS2**. This setting should be retained if possible. You should only set one of the two voltages if the automatic setting does not work and you know the exact specifications of your memory card.

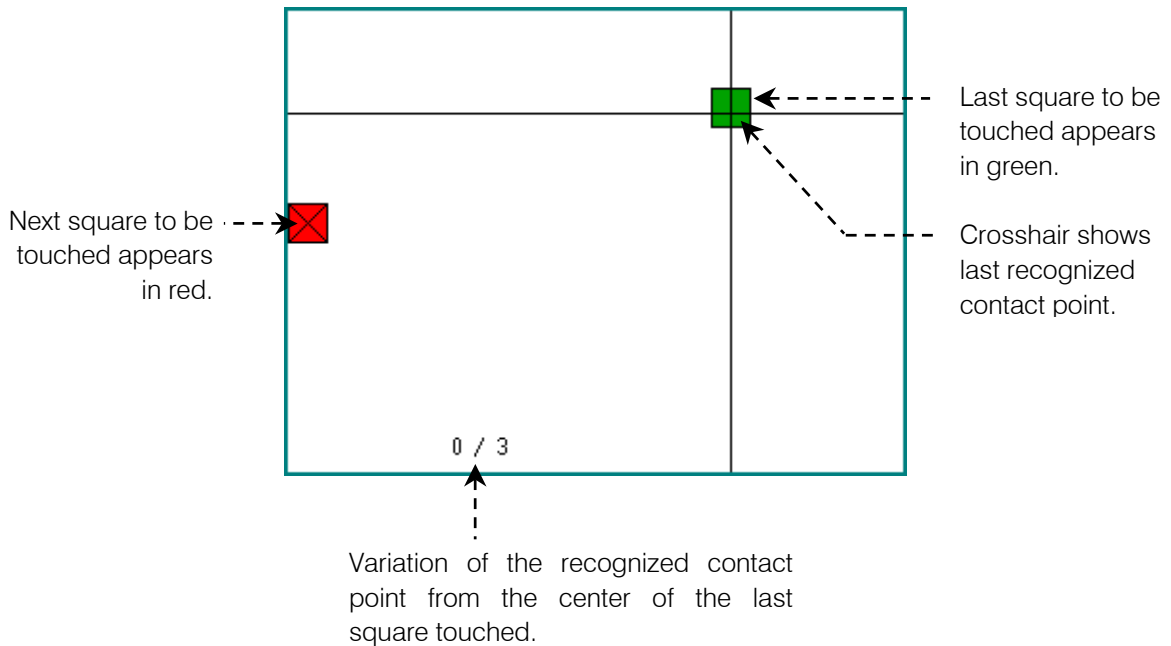
5.2.5 Service

Access to the service functions is password-protected and only accessible to Metrohm service technicians. We recommend that you have your Titrand system serviced by **Metrohm-Service** at regular intervals. You can automatically monitor the **time interval** after which the Titrand system needs to be serviced again (see *Section 3.12.5*).

5.2.6 Touch screen test

With the Touch screen test you can check the function of the Touch screen. A calibration is not possible with this test. In case the Touch screen does not work correctly anymore, it has to be replaced. For that please contact your Metrohm agency.

- ☞ Press **[Touch screen test]**.
- ☞ A red square now appears at various locations on the display in succession. You should try to touch the center of this square as exactly as possible in a suitable way (see *Section 3.1.3*). The contact point which is actually recognized is indicated by a crosshair:



- ☞ You can use **[Back]** to switch back again step by step.
- ☞ When you have checked all the display areas a list of **fixed keys** appears; you should touch them in any sequence. If they function correctly the request will always change to an appropriate message (e. g. **PRINT ok**).
- ☞ You can use **[Home]** to end the Touch screen test at any time or to conclude it.

5.2.7 Software update

With the Touch Control you can carry out an update of the instrument program or load a new dialog language. The instrument program (firmware) of the control device (Titrandu, USB Sample Processor etc.) can be updated with both the Touch Control and the PC Control.

The procedure for carrying out an update or a new installation of the PC Control software is described in Section 2.1.2.



Note!

It is essential that the control software (Touch Control or PC Control) is updated first and then the instrument program of the control device (Titrandu, USB Sample Processor etc.).

Touch Control and PC Control must always be updated at the same time as the control devices.

Loading a new dialog language (Touch Control only)



Note!

Only **one additional language** can be installed besides **English as the standard language**. If there is already a second language installed, it will be overwritten.

☞ In the **System/Diagnosis/Software update** menu select Touch Control under **Device**. In the selection list **Update type**, select the item **Second language** and confirm with **[Continue]**.

☞ Under **Binary file**, open the list with the program files on the memory card. The file name has the following structure:

Touch Control – Dialog language: 5xxxz1yy.BIN
 xxx = Touch Control version (device number)
 yy = 10 or higher (program version)
 z = 1 (German), 2 (French), 5 (Spanish)

Take care that the device and version numbers are correctly assigned.

☞ Select the required program file and press **[Select]**.

☞ Confirm the selected language file with **[Continue]**.

☞ Start loading the language with the **[Start]** fixed key. Further steps are shown in the dialog.

☞ A backup request appears. Confirm the process with **[Yes]**; the process is canceled with **[No]** and you have the possibility of saving your data.

☞ At the end of the update you must switch off the Touch Control and then switch it on again after a few seconds. A RAM initialization is carried out automatically (see *Section 5.3.2*). This takes some time.

Update of Titrando (PC Control and Touch Control)

☞ Select the Titrando to be updated in the menu **System/Diagnosis/Software update** under **Device** and press **[Continue]**.

☞ **[File]** accesses the selection of the program files. The file name has the following structure:

Titrandoo – program: 5xxx00yy.BIN
 xxx = Titrando version (device number)
 yy = 10 or higher (program version)

Take care that the device and version numbers are correctly assigned.

☞ Select the required program file with **[Open]**.

☞ Start the update with the **[Start]** fixed key. Further steps are shown in the dialog.

If the Titrando is updated from the Touch Control then the menu guidance is slightly different from that described above.

PC Control:

- ☞ When the update has been completed you must shut down the PC Control software. This is done by pressing **[Back]** or **[Home]** and confirming the following message with the request for a restart with **[OK]**. The PC Control program ends automatically.
- ☞ Restart PC Control.

Touch Control:

- ☞ When the update has been finished you must switch off the Touch Control, wait a few seconds, and then switch it on again.

Update of USB Sample Processor (PC Control and Touch Control)

- ☞ Select the USB Sample Processor to be updated in the menu **System/Diagnosis/Software update** under **Device** and press **[Continue]**.
- ☞ **[File]** accesses the selection of the program files. The file name has the following structure:

USB Sample Processor – program: 5xxx00yy .BIN
xxx = USB Sample Processor (device number)
yy = 10 or higher (program version)

Take care that the device and version numbers are correctly assigned.

- ☞ Select the required program file with **[Open]**.
- ☞ Start the update with the **[Start]** fixed key. Further steps are shown in the dialog.

If the USB Sample Processor is updated from the Touch Control then the menu guidance is slightly different from that described above.

PC Control:

- ☞ When the update has been completed you must shut down the PC Control software. This is done by pressing **[Back]** or **[Home]** and confirming the following message with the request for a restart with **[OK]**. The PC Control program ends automatically.
- ☞ Restart PC Control.

Touch Control:

- ☞ When the update has been finished you must switch off the Touch Control, wait a few seconds, and then switch it on again.

System file (Touch Control only)

- ☞ If you want to install new devices, e. g. balances or printers, for which there are no drivers in the control software you can load them by using this function. The procedure is identical to the update of the Touch Control.

5.2.8 822 Curve Simulator

The 822 Curve Simulator can be used as a diagnosis tool for checking the recording of the titration curves and their evaluation. Titration methods can be carried out and simulated measuring curves recorded without the actual presence of a measuring solution.

Details about the connection and operation of this instrument are given in the appropriate Instructions for Use.

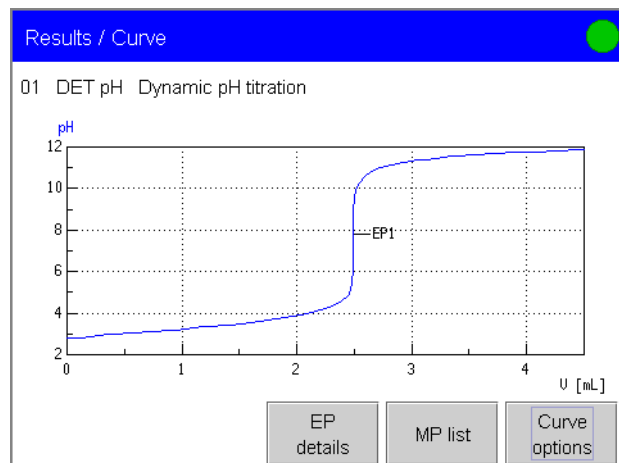
Please note that such a simulation requires that a correctly configured Dosimat or Dosino must be connected. A normal titration method is started. This means that the exchange or dosing unit should be emptied or the corresponding buret tip should be placed in a sufficiently large collection vessel.

Connection

- ☞ Switch off the Touch Control or pull out the Titrande mains cable or the USB plug at the PC (PC Control).
- ☞ First connect the analog output of the curve simulator with the electrode input "Ind." of the Titrande. Use the **6.2116.020** Cable with F-plugs at both ends.
- ☞ The 822 Curve Simulator is connected to the MSB port of the Titrande used. Take care that the dosing device is always the last device behind the curve simulator in as short a chain of MSB devices as possible (e. g. Titrande-MSB – Stirrer – 822 Curve Simulator – dosing device).
- ☞ If the internal dosing drive of the Titrande is used then the 822 Curve Simulator has to be connected to MSB port 2 of the Titrande. Switch on the Touch Control or start the PC Control and activate the checkbox "**Send dosing signals to MSB2**" under **System/Diagnosis/822 Curve Simulator**. Confirm the modification with **[Set]**. This copies the dosing signals to MSB port 2. Please note that this status can only be **deactivated** by a system restart.
- ☞ Switch on the Touch Control again or reinsert the mains plug and start the PC Control software.

Simulation of a titration

- ☞ For the following example of a simulation you should load the **Tutorial** method from the examples of methods stored under **Card 1/Examples**.
- ☞ Rotate the curve selection switch on the 822 Curve Simulator to curve **0** (Titration of an acid with a base).
- ☞ Start the titration with **[Start]**.
- ☞ When the titration has been carried out you will obtain the following example of a curve under **Results/Curve**:



5.2.9 Remove PCMCIA card 1/2

As long as the Touch Control is not accessing the data on the inserted memory card for loading or storing you can remove and insert the memory card without any problems with the Touch Control switched on.

This option offers additional data protection as it ensures that the data to be stored is completely written onto the card before the power supply to the card is switched off.

Remove the card as soon as the appropriate message appears:

The PCMCIA card can be removed now

5.3 Maintenance

5.3.1 Changing the batteries (Touch Control only)

The Touch Control indicates that its batteries need changing with the message "Battery low". Please note that the current date and time will be reset to 1.1.2000 and 00:00:00 respectively.

Proceed as follows:

- ☞ Switch off the Touch Control.
- ☞ Remove the three fastening screws of the protective cover on the base of the housing:

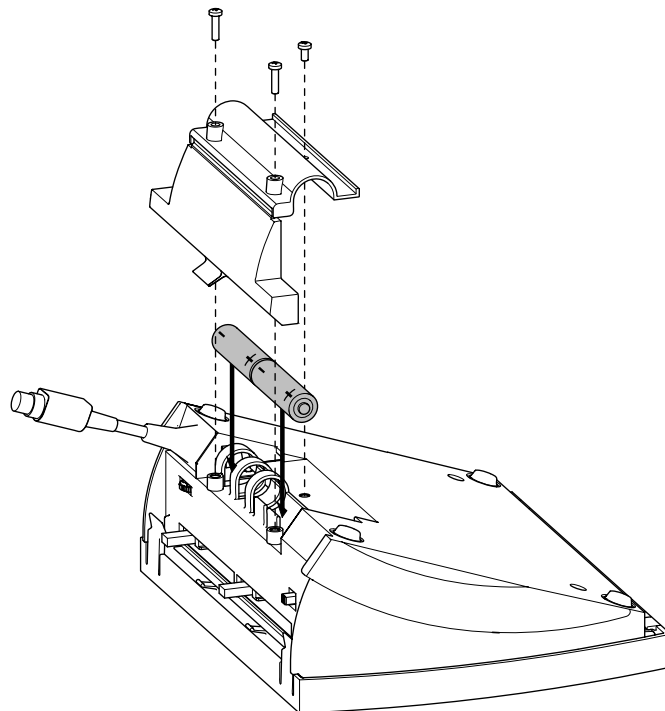


Fig. 5.1: Changing the batteries for Touch Control

- ☞ Exchange the existing batteries for two new 1.5 V alkaline manganese batteries, type LR6/AA/AM3 (Metrohm Order number 6.2133.010).
- ☞ Make sure that the poles of the batteries are positioned correctly! The correct arrangement is shown in the battery compartment.
- ☞ Reattach the protective cover to the rear panel with the three screws and close it.
- ☞ Switch on the Touch Control and reset the date and time (see Section 3.7.2).



5.3.2 RAM initialization (RAM Init, Touch Control only)

In very rare cases excessive interference could affect the functions of the processor and cause a program crash. In this case the RAM sector must be initialized. RAM initialization is also the only way of making the system accessible again if it is impossible for a user to log in because, for example, even the Administrator has forgotten the password or no Administrator has been defined (see *Section 3.7.5*).

**Attention!**

If you carry out a **RAM initialization** (RAM Init) then **all user data will be lost**. The contents of the internal memory will be deleted. The system will return to the "factory settings". An additionally installed language continues to exist.

**Note!**

You should make a **backup** at **regular intervals** in order to avoid data loss. For the Touch Control we recommend – depending on how frequently you alter methods or system settings – making a backup every week to every month. For the PC Control software the period should be in accordance with that usually used for data security backups in your company.

For RAM initialization proceed as follows:

- ☞ Switch off the Touch Control with the ON/OFF switch **11**.
- ☞ **Switch on** the Touch Control again with the ON/OFF switch **11** while keeping the **contrast controller 14 pressed down**. You can release the contrast controller when you hear an **acoustic signal** (beep).
- ☞ To confirm the RAM initialization **press** the **contrast controller twice**.

The RAM will be checked and initialized.

If you do not confirm the RAM initialization within 10 seconds of hearing the acoustic signal the process will be stopped and the Touch Control will be switched on without a RAM initialization.

6 Appendix

In this section you will find the most important technical data for the Touch Control, a list of standard accessories and optional accessories for the Touch Control and PC Control software as well as the warranty and declarations of conformity.

6.1 Technical data

Provided that nothing to the contrary is mentioned, the published values represent typical technical data for the Touch Control.

6.1.1 Touch screen

<i>Display</i>	¼ VGA color display, 320 pixel x 240 pixel, 12 cm x 9 cm
<i>Touch panel</i>	analog resistive

6.1.2 Interfaces

Titrand connection

<i>Cable</i>	8-pole, 70 cm, shielded, Mini-DIN plug with lock
--------------	--

PCMCIA card slot

<i>Card slot</i>	PCMCIA (Personal Computer Memory Card International Association) ATA Card type I/II
<i>Cards</i>	FlashCards for storing methods, determinations, sample data silos, result silos and backups (PCMCIA cards or CompactFlash cards with CompactFlash adapter)

6.1.3 Power supply

<i>Voltage</i>	±12 V, +5 V
<i>Power consumption</i>	5 W
<i>Batteries</i>	2 x 1.5 V alkaline manganese or lithium, type LR6/AA/AM3

6.1.4 Safety specifications

<i>Construction and testing</i>	According to EN/IEC/UL 61010-1, CSA-C22.2 No. 61010-1, protection class III
<i>Safety information</i>	The documentation contains safety instructions which have to be followed by the user in order to ensure safe operation of the instrument.

6.1.5 Electromagnetic compatibility (EMC)

Emission Standards fulfilled:
- EN/IEC 61326-1
- EN/IEC 61000-6-3
- EN 55022 / CISPR 22

Immunity Standards fulfilled:
- EN/IEC 61326-1
- EN/IEC 61000-6-2
- EN/IEC 61000-4-2
- EN/IEC 61000-4-3

6.1.6 Ambient temperature

Nominal working range +5 °C...+40 °C (at max. 85% rel. humidity)
Storage -20 °C...+60 °C
Transport -40 °C...+60 °C

6.1.7 Dimensions

Housing material Polybutylene terephthalate (PBT)
Film material Polyester
Width 210 mm
Height 83 mm
Depth approx. 198 mm
Weight 1437 g

6.2 Remote box

The 6.2148.010 Remote box allows devices to be controlled which cannot be connected directly to the MSB interface of the Titrando, e. g. Level Control 849. The connection of the Remote box is described in the Installation Instructions for the Titrando.

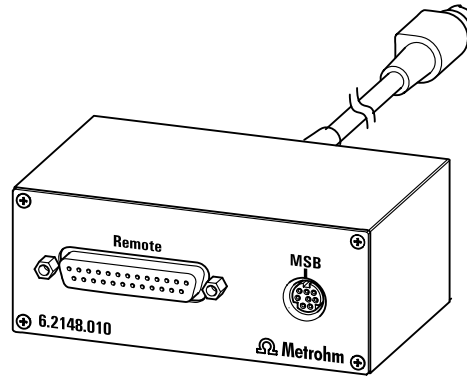


Fig. 6.1: View of the connections of the optional 6.2148.010 Remote box

6.2.1 Pin occupancy of the remote connection at the Remote box

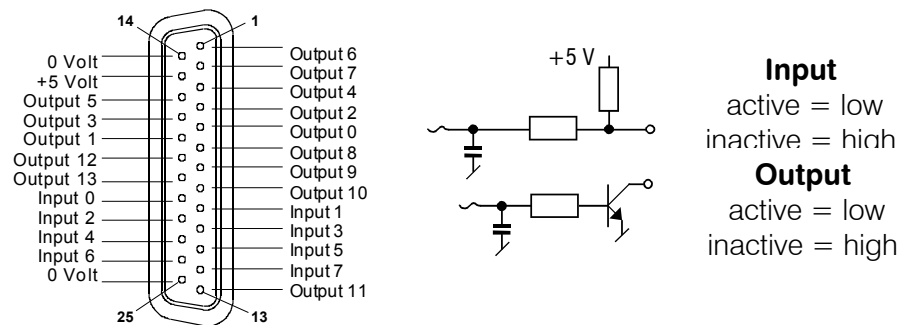


Fig. 6.2: Pin occupancy at remote interface

The following applies for all outputs: $V_{CE0} = 40 \text{ V}$
 $I_C = 20 \text{ mA}$
 $t_{\text{pulse}} > 100 \text{ ms}$

6.2.2 Functions of the individual remote lines

Name	Pin.	Function
Input 0	21	START On activation the current method is started. $t_{\text{pulse}} > 100 \text{ ms}$
Input 1	9	STOP On activation the current determination is halted (Stop). $t_{\text{pulse}} > 100 \text{ ms}$
Input 3	10	CANCEL On activation the current command in the determination run will be halted. $t_{\text{pulse}} > 100 \text{ ms}$
Input 4	23	- Not occupied, can be used for scanning the Sample Processor (sample in work position).
Input 5	11	- Not occupied.
Output 0	5	READY The Titrando is ready to receive a start signal.
Output 1	18	Cond. OK Line will be set when conditioning is OK for SET and KFT titrations. The line remains set until the titration itself is started with [Start] .
Output 2	4	TITRATION The Titrando is carrying out a data producing sequence.
Output 3	17	EOD End of Determination Pulse ($t_{\text{pulse}} = 200 \text{ ms}$) after a determination or after a buffer/standard during calibration using a Sample Processor.
Output 4	3	- Not occupied.
Output 5	16	ERROR Line is set for error message display.
Output 6	1	- Not occupied.
Output 7	2	WARNING Line is set for warning message display.
Voltage:		
+5 V	15	$I \leq 40 \text{ mA}$
0 V	14/25	0 V: active (low), 5 V: inactive

6.3 RS-232/USB Box

If Touch Control is used then the 6.2148.020 RS-232/USB Box allows devices with a serial RS-232 interface to be directly connected to the Titrando. Such a device could be a balance or computer for data transmission.

The connection of devices via the RS-232/USB Box is described in the Installation Instructions for the Titrando.

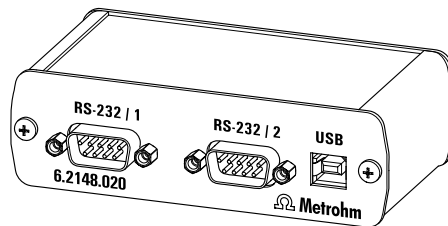


Fig. 6.3: View of the connections of the optional RS-232/USB Box

6.3.1 RS-232 parameters

The RS-232/USB Box makes the **RS-232 interfaces 1 and 2 (RS-232 1 and RS-232 2)** available to the Titrando. The configuration of these interfaces can be carried out in the device manager under **Serial ports** (PC Control) or **RS-232/USB Box** (Touch Control) respectively (see Section 3.10.10). The following list shows the default parameters for Touch Control and PC Control in bold type:

Baud rate:	1200, 2400, 4800, 9600 , 19200, 38400, 57600, 115200
Data bits:	7, 8 Bits
Parity:	even , odd, none
Stop bits	1,2 bits
Handshake:	none, software(XOn/XOff), hardware(DTR/CTS)

6.3.2 RS-232 pin occupancy

RS-232 connection: D-sub 9-pole, male, full

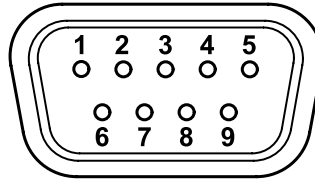


Fig. 6.4: View of the RS-232 connections on the RS-232/USB Box

Pin 1:	-	
Pin 2:	RxD ←	Data reception (Receive Data)
Pin 3:	TxD →	Data transmission (Transmit Data)
Pin 4:	DTR →	Ready to receive (Data Terminal Ready)
Pin 5:	GND ⊥	Zero voltage, reference potential (ground)
Pin 6:	DSR ←	Only used for diagnosis (Data Set Ready)
Pin 7:	RTS →	Transmitter to send (Request To Send)
Pin 8:	CTS ←	Receiver ready to receive (Clear To Send)
Pin 9:	-	

6.4 Stored buffer series for CAL pH

For automatic buffer recognition during pH calibration the temperature-dependent pH values of several common pH buffers are stored in the system. Apart from the Metrohm buffer solutions other reference and technical buffers are also included in the tables.

The following tables provide an overview of the stored pH(T) series:

The pH values printed in bold are the values at the reference temperature of the particular buffer set.

The pH values marked with ¹⁾ are interpolated or extrapolated values, all the others correspond to the manufacturer's specifications.

Temp. (°C)	Metrohm			NIST (according to DIN standard 19266, 2000)				
	Met4 pH 4.00	Met7 pH 7.00	Met9 pH 9.00	NIST1 pH 1	NIST4 pH 4	NIST7 pH 7	NIST9 pH 9	NIST13 pH 13
0	3.99	7.11	9.27	-	4.010	6.984	9.464	13.423
5	3.99	7.08	9.18	1.668	4.004	6.950	9.392	13.207
10	3.99	7.06	9.13	1.670	4.001	6.922	9.331	13.003
15	3.99	7.04	9.08	1.672	4.001	6.900	9.277	12.810
20	3.99	7.02	9.04	1.676	4.003	6.880	9.228	12.627
25	4.00	7.00	9.00	1.680	4.008	6.865	9.184	12.454
30	4.00	6.99	8.96	1.685	4.015	6.853	9.144	12.289
35	4.01	6.98	8.93	1.691	4.025	6.843	9.107	12.133
40	4.02	6.98	8.90	1.697	4.036	6.837	9.076	11.984
45	4.03	6.97	8.87	1.704	4.049	6.834	9.046	11.841
50	4.04	6.97	8.84	1.712	4.064	6.833	9.018	11.705
55	4.06	6.97	8.81	1.715	4.075	6.834	8.985	11.574
60	4.07	6.97	8.79	1.723	4.091	6.836	8.962	11.449
65	4.09	6.98	8.76	1.732 ¹⁾	4.108 ¹⁾	6.840 ¹⁾	8.941 ¹⁾	-
70	4.11	6.98	8.74	1.743	4.126	6.845	8.921	-
75	4.13	6.99	8.73	1.754 ¹⁾	4.145 ¹⁾	6.852 ¹⁾	8.902 ¹⁾	-
80	4.15	7.00	8.71	1.766	4.164	6.859	8.885	-
85	4.18	7.00	8.70	1.778 ¹⁾	4.185 ¹⁾	6.867 ¹⁾	8.867 ¹⁾	-
90	4.20	7.01	8.68	1.792	4.205	6.877	8.850	-
95	4.23	7.02	8.67	1.806	4.227	6.886	8.833	-

Temp. (°C)	DIN (according to DIN standard 19267, 1978)					
	DIN1 pH 1	DIN3 pH 3	DIN4 pH 4	DIN7 pH 7	DIN9 pH 9	DIN12 pH 12
0	1.08	-	4.67	6.89	9.48	-
5	1.08 ¹⁾	-	4.66 ¹⁾	6.86 ¹⁾	9.43 ¹⁾	-
10	1.09	3.10	4.66	6.84	9.37	13.37
15	1.09 ¹⁾	3.08 ¹⁾	4.65 ¹⁾	6.82 ¹⁾	9.32 ¹⁾	13.15 ¹⁾
20	1.09	3.07	4.65	6.80	9.27	12.96
25	1.09	3.06	4.65	6.79	9.23	12.75
30	1.10	3.05	4.65	6.78	9.18	12.61
35	1.10 ¹⁾	3.05 ¹⁾	4.66 ¹⁾	6.77 ¹⁾	9.13 ¹⁾	12.44 ¹⁾
40	1.10	3.04	4.66	6.76	9.09	12.29
45	1.10 ¹⁾	3.04 ¹⁾	4.67 ¹⁾	6.76 ¹⁾	9.04 ¹⁾	12.13 ¹⁾
50	1.11	3.04	4.68	6.76	9.00	11.98
55	1.11 ¹⁾	3.04 ¹⁾	4.69 ¹⁾	6.76 ¹⁾	8.97 ¹⁾	11.84 ¹⁾
60	1.11	3.04	4.70	6.76	8.92	11.69
65	1.11 ¹⁾	3.04 ¹⁾	4.71 ¹⁾	6.76 ¹⁾	8.90 ¹⁾	11.56 ¹⁾
70	1.11	3.04	4.72	6.76	8.88	11.43
75	1.12 ¹⁾	3.04 ¹⁾	4.74 ¹⁾	6.77 ¹⁾	8.86 ¹⁾	11.30 ¹⁾
80	1.12	3.05	4.75	6.78	8.85	11.19
85	1.12 ¹⁾	3.06 ¹⁾	4.77 ¹⁾	6.79 ¹⁾	8.83 ¹⁾	11.08 ¹⁾
90	1.13	3.07	4.79	6.80	8.82	10.99
95	-	-	-	-	-	-

Temp. (°C)	Fisher				Fluka Basel		
	Fis2 pH 2	Fis4 pH 4	Fis7 pH 7	Fis10 pH 10	FBS4 pH 4	FBS7 pH 7	FBS9 pH 9
0	-	4.01	7.13	10.34	4.01	7.11	9.20
5	1.98	3.99	7.10	10.26	4.00	7.08	9.15
10	1.98	4.00	7.07	10.19	4.00	7.05	9.10
15	2.02	3.99	7.05	10.12	4.00	7.02	9.05
20	2.00	4.00	7.02	10.06	4.00	7.00	9.00
25	2.00	4.00	7.00	10.00	4.01	6.98	8.96
30	2.00	4.01	6.99	9.94	4.01	6.97	8.91
35	2.02	4.02	6.98	9.90	4.02	6.96	8.88
40	2.01	4.03	6.97	9.85	4.03	6.95	8.84
45	2.01	4.04 ¹⁾	6.97 ¹⁾	9.81 ¹⁾	4.04	6.94	8.80
50	2.01	4.06	6.97	9.78	4.06	6.94	8.77
55	-	4.07 ¹⁾	6.97 ¹⁾	9.74 ¹⁾	4.07	6.93	8.74
60	-	4.09	6.98	9.70	4.09	6.93	8.71
65	-	4.11 ¹⁾	6.99 ¹⁾	9.68 ¹⁾	4.11 ¹⁾	6.93 ¹⁾	8.69 ¹⁾
70	-	4.13 ¹⁾	7.00 ¹⁾	9.65 ¹⁾	4.13	6.94	8.67
75	-	4.14 ¹⁾	7.02 ¹⁾	9.63 ¹⁾	4.14 ¹⁾	6.94 ¹⁾	8.65 ¹⁾
80	-	4.16 ¹⁾	7.03 ¹⁾	9.62 ¹⁾	4.16	6.95	8.63
85	-	4.18 ¹⁾	7.06 ¹⁾	9.61 ¹⁾	4.18 ¹⁾	6.96 ¹⁾	8.61 ¹⁾
90	-	4.21 ¹⁾	7.08 ¹⁾	9.60 ¹⁾	4.21	6.97	8.60
95	-	4.23 ¹⁾	7.11 ¹⁾	9.60 ¹⁾	4.23 ¹⁾	6.98 ¹⁾	8.59 ¹⁾

Temp. (°C)	Mettler Toledo					Beckman		
	MT2 pH 2	MT4 pH 4	MT7 pH 7	MT9 pH 9	MT11 pH 11	Bec4 pH 4	Bec7 pH 7	Bec10 pH 10
0	2.03 ¹⁾	4.01 ¹⁾	7.12 ¹⁾	9.52 ¹⁾	11.90 ¹⁾	4.00	7.12	10.32
5	2.02	4.01	7.09	9.45	11.72	4.00	7.09	10.25
10	2.01	4.00	7.06	9.38	11.54	4.00	7.06	10.18
15	2.00	4.00	7.04	9.32	11.36	4.00	7.04	10.12
20	2.00	4.00	7.02	9.26	11.18	4.00	7.02	10.06
25	2.00	4.01	7.00	9.21	11.00	4.00	7.00	10.01
30	1.99	4.01	6.99	9.16	10.82	4.01	6.99	9.97
35	1.99	4.02	6.98	9.11	10.64	4.02	6.99	9.93
40	1.98	4.03	6.97	9.06	10.46	4.03	6.98	9.89
45	1.98	4.04	6.97	9.03	10.28	4.05	6.98	9.86
50	1.98	4.06	6.97	8.99	10.10	4.06	6.97	9.83
55	1.98 ¹⁾	4.08 ¹⁾	6.98 ¹⁾	8.96 ¹⁾	-	4.08	6.98	-
60	1.98 ¹⁾	4.10 ¹⁾	6.98 ¹⁾	8.93 ¹⁾	-	4.09	6.98	-
65	1.98 ¹⁾	4.13 ¹⁾	6.99 ¹⁾	8.90 ¹⁾	-	4.11	6.99	-
70	1.99 ¹⁾	4.16 ¹⁾	7.00 ¹⁾	8.88 ¹⁾	-	4.12	6.99	-
75	1.99 ¹⁾	4.19 ¹⁾	7.02 ¹⁾	8.85 ¹⁾	-	4.14	7.00	-
80	2.00 ¹⁾	4.22 ¹⁾	7.04 ¹⁾	8.83 ¹⁾	-	4.16	7.00	-
85	2.00 ¹⁾	4.26 ¹⁾	7.06 ¹⁾	8.81 ¹⁾	-	4.18	7.01	-
90	2.00 ¹⁾	4.30 ¹⁾	7.09 ¹⁾	8.79 ¹⁾	-	4.19	7.02	-
95	-	4.35 ¹⁾	7.12 ¹⁾	8.77 ¹⁾	-	4.21	7.03	-

Temp. (°C)	Radiometer			Baker			
	Rad4.01 pH 4.01	Rad7.00 pH 7	Rad9.18 pH 9.18	Bak4 pH 4.00	Bak7 pH 7.00	Bak9 pH 9.00	Bak10 pH 10.00
0	4.000	7.118	9.464	4.00	7.13	9.23	10.30
5	3.998	7.087	9.395	4.00 ¹⁾	7.09 ¹⁾	9.17 ¹⁾	10.24 ¹⁾
10	3.997	7.059	9.332	4.00	7.05	9.10	10.17
15	3.998	7.036	9.276	4.00 ¹⁾	7.03 ¹⁾	9.05 ¹⁾	10.11 ¹⁾
20	4.001	7.016	9.225	4.00	7.00	9.00	10.05
25	4.005	7.000	9.180	4.00 ¹⁾	6.98 ¹⁾	8.96 ¹⁾	10.00
30	4.011	6.987	9.139	4.01	6.98	8.91	9.96
35	4.018	6.977	9.102	4.02 ¹⁾	6.98 ¹⁾	8.88 ¹⁾	9.93 ¹⁾
40	4.027	6.970	9.068	4.03	6.97	8.84	9.89
45	4.038	6.965	9.038	4.04 ¹⁾	6.97 ¹⁾	8.81 ¹⁾	9.86 ¹⁾
50	4.050	6.964	9.011	4.05	6.96	8.78	9.82
55	4.064	6.965	8.985	4.07 ¹⁾	6.96 ¹⁾	8.76 ¹⁾	9.79 ¹⁾
60	4.080	6.968	8.962	4.08	6.96	8.73	9.76
65	4.097	6.974	8.941	4.10 ¹⁾	6.97 ¹⁾	8.71 ¹⁾	9.74 ¹⁾
70	4.116	6.982	8.921	4.12	6.97	8.69	9.72
75	4.137	6.992	8.900	4.14 ¹⁾	6.98 ¹⁾	8.68 ¹⁾	9.70 ¹⁾
80	4.159	7.004	8.885	4.16	6.98	8.66	9.68
85	4.183	7.018	8.867	4.19 ¹⁾	6.99 ¹⁾	8.64 ¹⁾	9.66 ¹⁾
90	4.210	7.034	8.850	4.21	7.00	8.62	9.64
95	4.240	-	-	-	-	-	-

Temp. (°C)	Hamilton DURACAL				Precisa		
	Ham4.01 pH 4.01	Ham7.00 pH 7.00	Ham9.21 pH 9.21	Ham10.01 pH10.01	Pre4 pH 4.00	Pre7 pH 7.00	Pre9 pH 9.00
0	-	-	-	-	3.99	7.11	9.27
5	4.01	7.09	9.45	10.19	3.99	7.08	9.18
10	4.00	7.06	9.38	10.15	3.99	7.06	9.13
15	4.00	7.04	9.32	10.11	3.99	7.04	9.08
20	4.00	7.02	9.26	10.06	3.99	7.02	9.04
25	4.01	7.00	9.21	10.01	4.00	7.00	9.00
30	4.01	6.99	9.16	9.97	4.00	6.99	8.96
35	4.02	6.98	9.11	9.92	4.01	6.98	8.93
40	4.03	6.97	9.06	9.86	4.02	6.98	8.90
45	4.04	6.97	9.03	9.83	4.03	6.97	8.87
50	4.06	6.97	8.99	9.79	4.04	6.97	8.84
55	-	-	-	-	4.06	6.97	8.81
60	-	-	-	-	4.07	6.97	8.79
65	-	-	-	-	4.09	6.98	8.76
70	-	-	-	-	4.11	6.98	8.74
75	-	-	-	-	4.13	6.99	8.73
80	-	-	-	-	4.15	7.00	8.71
85	-	-	-	-	4.18	7.00	8.70
90	-	-	-	-	4.20	7.01	8.68
95	-	-	-	-	4.23	7.02	8.67

Temp. (°C)	Merck Titrisol				
	Mer2 pH 2	Mer4 pH 4	Mer7 pH 7	Mer9 pH 9	Mer12 pH 12
0	2.01	4.05	7.13	9.24	12.58
5	2.01	4.04	7.07	9.16	12.41
10	2.01	4.02	7.05	9.11	12.26
15	2.00	4.01	7.02	9.05	12.10
20	2.00	4.00	7.00	9.00	12.00
25	2.00	4.01	6.98	8.95	11.88
30	2.00	4.01	6.98	8.91	11.72
35	2.00	4.01	6.96	8.88	11.67
40	2.00	4.01	6.95	8.85	11.54
45	2.00 ¹⁾	4.00 ¹⁾	6.95 ¹⁾	8.82 ¹⁾	11.44 ¹⁾
50	2.00	4.00	6.95	8.79	11.33
55	2.00 ¹⁾	4.00 ¹⁾	6.95 ¹⁾	8.76 ¹⁾	11.19 ¹⁾
60	2.00	4.00	6.96	8.73	11.04
65	2.00 ¹⁾	4.00 ¹⁾	6.96 ¹⁾	8.715 ¹⁾	10.97 ¹⁾
70	2.01	4.00	6.96	8.70	10.90
75	2.01 ¹⁾	4.00 ¹⁾	6.96 ¹⁾	8.68 ¹⁾	10.80 ¹⁾
80	2.01	4.00	6.97	8.66	10.70
85	2.01 ¹⁾	4.00 ¹⁾	6.98 ¹⁾	8.65 ¹⁾	10.59 ¹⁾
90	2.01	4.00	7.00	8.64	10.48
95	-	4.00 ¹⁾	7.02 ¹⁾	-	-

Temp. (°C)	Merck CertiPUR (25 °C)			
	MerC4.01 pH 4.01	MerC7.00 pH 7.00	MerC9.00 pH 9.00	MerC10.00 pH 10.00
0	-	-	-	-
5	4.00	7.09	9.22	10.22
10	4.00	7.06	9.16	10.16
15	4.00	7.04	9.10	10.10
20	4.00	7.02	9.05	10.05
25	4.01	7.00	9.00	10.00
30	4.01	6.98	8.96	9.94
35	4.03	6.98	8.93	9.90
40	4.03	6.97	8.89	9.86
45	4.05	6.97	8.87	9.80
50	4.06	6.97	8.84	9.73
55	-	-	-	-
60	-	-	-	-
65	-	-	-	-
70	-	-	-	-
75	-	-	-	-
80	-	-	-	-
85	-	-	-	-
90	-	-	-	-
95	-	-	-	-

When using Merck CertiPUR (20 °C) buffers, you have to select the buffer type "Merck Titrisol".

6.5 Liquid handling – schematic process

6.5.1 Port definitions of the dosing unit

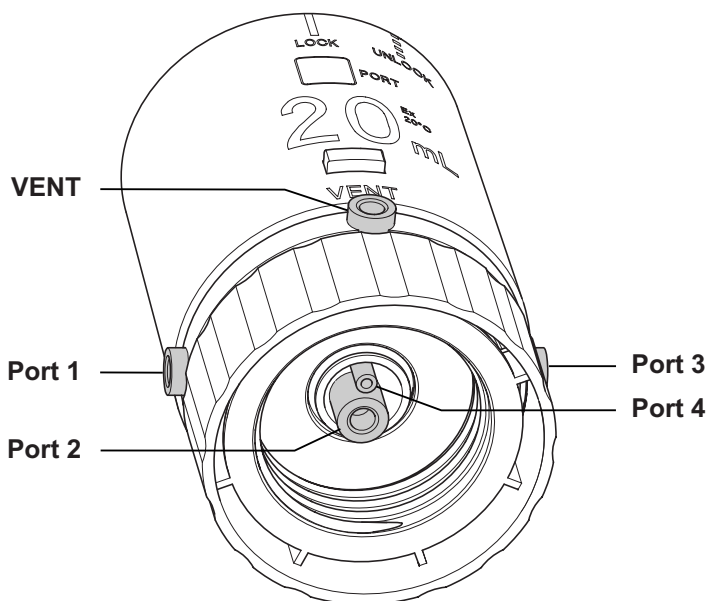


Fig. 6.5: Port occupancy of the Dosing unit

- VENT** – is intended for venting the storage bottle and is normally fitted with an adsorber tube (filled with a drying agent).
- Port 1** – is side-mounted; its default definition is as dosing port 1.
- Port 2** – is located at the base; its default definition is as filling port and it is normally fitted with a riser tube.
- Port 3** – is side-mounted; its default definition is as dosing port 2.
- Port 4** – is located at the base; its default definition is as air inlet port for emptying the tubing system.

6.5.2 Pipetting equipment

Together with an 800 Dosino as the dosing drive (or "pipetting pump") the USB Sample Processor is exceedingly suitable for pipetting liquids in a volume range between 0.1 and 10 mL.

Necessary equipment

- USB Sample Processor with 786 Swing Head
- Swing Head with transfer head (e. g. 6.1462.030 or 6.1462.040)
- 800 Dosino with 2 mL, 5 mL, 10 mL or 20 mL dosing unit
- 6.1562.020 Pipetting tubing (3 mL) or 6.1562.100 (10 mL) with drawn-out tip
- Any sample rack
- Possibly 6.2001.070 Support Stand with titration cell

6.5.3 Pipetting sequences

Principle

Measuring out the liquid to be pipetted takes place in the pipetting tubing, which is filled with a carrier liquid (preferably water). In order to avoid carryover or mixing an air bubble (separating bubble) must be inserted between the sample and the carrier liquid. The tubing tip should be drawn out by hand to form a fine point.

A Dosino drive is used to transfer the liquids to the tubing. The pipetting tubing is attached to Port 1 of the dosing unit. The dosing unit is mounted on a storage bottle containing the carrier liquid. This can be refilled via filling Port 2 of the dosing unit. The carrier liquid can also be used for rinsing and diluting the sample.

Numerous pipetting sequences are possible. The following conditions must always be observed:

- The sample must always be measured out in the pipetting tubing; it must never enter the dosing unit cylinder.
- The sample should always be aspirated after the dosing cylinder has been ejected.
- The difference in level between the surface of the sample liquid and that of the carrier liquid in the dosing cylinder should be as small as possible.
- Aqueous sample solutions can be pipetted without having to rinse the tubing. Non-aqueous samples require the pipetting tubing to be rinsed with carrier liquid (same solvent as the sample) to avoid carryover.

Only the most necessary commands are mentioned in the following command sequence. A complete command sequence is defined in the **method template "SP Pipetting Ext. Position"** (see *Section 3.15.2*).

Preparing the dosing unit

The dosing unit must first be prepared, i.e. the filling tubing and pipetting tubing must be rinsed and completely filled. The preparation step is best carried out at an external position. The cylinder contents must then be ejected. This command sequence is best combined to a subsequence. This preparation step is only necessary at the beginning of a sample series. Therefore the subsequence is defined as **Start sequence** (see *Section 4.9.6*).

Command sequence:	MOVE	move to external position
	LIFT	move to work position
	PREP	prepare dosing device
	LQH	eject cylinder

These steps should be carried out before every sample series involving pipetting. Before each pipetting process the dosing unit cylinder contents must be completely ejected. This is the only way to achieve reproducible, accurate pipetting.

The titration cell can then be sucked off, rinsed and prepared with fresh solvent.

Pipetting

The pipetting procedure takes place in five steps:

- Eject cylinder contents (see above) and form separating bubble
- Move to sample
- Aspirate / Measure out sample
- Move to target
- Eject sample

These five Steps can be combined to a subsequence defined as **Sample sequence** (see *Section 4.9.6*).

Forming a separating bubble

In order to prevent the carrier liquid and sample solution from mixing, a separating bubble must be formed that occupies a length of at least 5 mm in the pipetting tubing. However, the separating bubble must also be measured out with sufficient accuracy. This is why a dosing unit with max. 20 mL cylinder capacity should be used for pipetting.

Command sequence:	LIFT	move to shift position
	LQH	aspirate air

Move to sample

The (dissolved or liquid) samples can be contained in open beakers on the rack or in sealed vials. In the latter case instead of the pipetting tubing a suitable injection needle should be connected to Dosino Port 1 with a normal piece of tubing (\varnothing 2 mm).

Command sequence:	MOVE	move to sample
	LIFT	move to work position

Aspirate sample

Aspiration of the sample should be carried out at a reduced filling rate (< 10 mL/min). The appropriate setting can be made in the liquid handling command under **Rate**.

With non-aqueous samples in particular an additional small air bubble should be drawn into the pipetting tip in order to prevent the sample solution from dripping.

Command sequence:	LQH	aspirate sample
	WAIT	pause
	LIFT	move to shift position
	LQH	aspirate air

Move to target

Before the pipetting tubing containing the measured-out sample is moved, the corresponding Dosino port must be closed. Ideally a change should be made to filling Port 2 as this certainly contains no air.

The titration cell should be filled with solvent before the sample is added so that the sample can be pipetted directly into the liquid (tip immersed).

Command sequence:	LQH	change port
	MOVE	move to titration cell
	LIFT	move to work position

Eject sample

The sample should be ejected at a reduced dosing rate (< 10 mL/min). The appropriate settings can be made in the liquid handling command under **Rate**.

Command sequence:	LQH	End volume
-------------------	-----	------------

Rinse

In order to keep sample solution carryover as low as possible, rinsing with solvent can be carried out after the sample has been ejected. This is particularly recommended for non-aqueous samples.

In preparation for the next pipetting process the cylinder should be completely ejected.

Command sequence:	LQH	fill or aspirate
	LQH	eject

6.6 Titration and measuring modes in the Titrando system

	<i>Device</i>							
	808	809	835	836	841	842	857	855
<i>DET</i>	•	•	•	•	–	–	•	•
<i>MET</i>	•	•	•	•	–	–	•	•
<i>SET</i>	•	•	•	•	•	• ¹⁾	•	•
<i>KFT</i>	–	–	•	•	•	–	•	–
<i>STAT</i>	–	–	•	•	–	• ¹⁾	•	•
<i>MEAS</i>	•	•	•	•	•	• ¹⁾	•	•
<i>MEAS Conc</i>	•	•	•	•	–	–	•	•
<i>CAL</i>	•	•	•	•	• ²⁾	• ²⁾	•	•
<i>DOS</i>	–	–	•	•	–	•	•	•

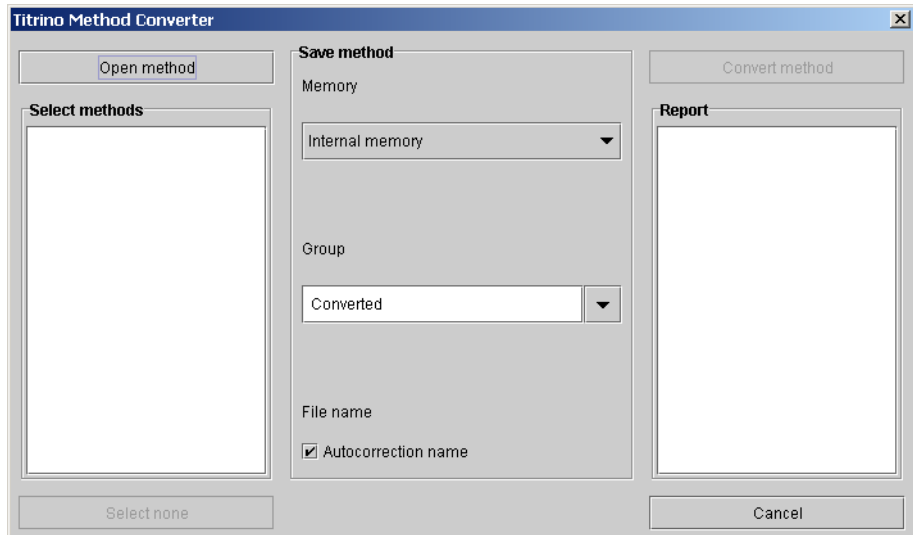
¹⁾ no U(pol), I(pol)

²⁾ no CAL Conc.

6.7 Import of Titrino methods (PC Control only)

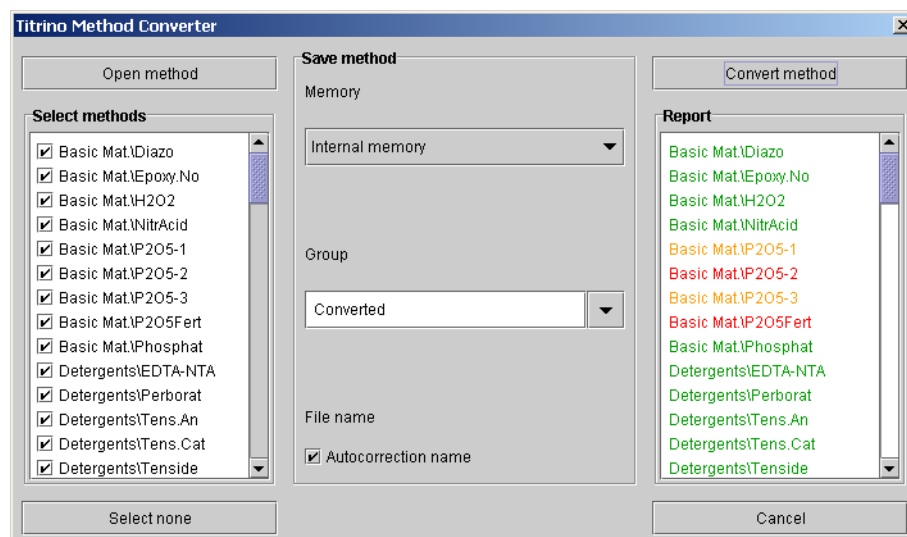
With the Titrino method converter you can import Titrino methods into the PC Control software.

- ☞ Use the Metrohm **VESUV** software to save the methods which are stored in the Titrino. The methods are stored in a .vmb file.
- ☞ In the **File** menu open the menu item **Import Methods...**



- ☞ Use **[Open method]** to open the **Vesuv backup file** dialog. Select the required .vmb file and open it. The methods are listed under **Select methods**. If the methods have been stored in folders in the Titrino then the folder will be shown in front of the method name and separated from it by "/".
- ☞ If you do not want to import all the methods in the backup file then you can deactivate the checkboxes for these methods. With **[Select none]** or **[Select all]** you can select either none or all of the methods in the list respectively.
- ☞ Under **Save method** select the **Memory** and **Group** in which the converted methods are to be stored. If the **Autocorrection name** function is switched on then invalid characters in method names will be replaced by "_".
- ☞ Start the conversion with **[Convert method]**. The conversion can be stopped at any time with **[Cancel]**.

Any messages produced during the conversion of the methods will be shown under **Report**.



The methods are shown in color. The colors have the following meanings:

- Green: conversion OK.
- Yellow: 1:1 not possible. The converted method must be checked.
- Red: conversion not possible.

If you click on the method name then all the messages referring to this method will be shown in a new dialog window. The following messages may be produced:

Conversion OK (green-marked methods)

- The method has been converted successfully.
- An old method file with the same name has been replaced.
- The method file has been renamed to: New method name

Check converted method (yellow-marked methods)

- Single commands could not be converted.
- The assignment to a temporary variable (C70 to C79) for TIP was ignored.
- The assignment of a temporary variable (C70 to C79) to a common variable is not possible.
- The assignment of a temporary variable (C70 to C79) to a statistics variable is not possible.
- A formula contains a temporary variable (C70 to C79). The variable has been replaced by -0.
- The assignment to a silo calculation variable (C24 to C27) has been ignored.
- The assignment of a silo calculation variable (C24 to C27) to a common variable is not possible.
- The assignment of a silo calculation variable (C24 to C27) to a statistics variable is not possible.
- A formula contains a silo calculation variable (C24 to C27). The variable has been replaced by -0.

- The assignment of sample identification 3 (C23) to a common variable is not possible.
- The assignment of sample identification 3 (C23) to a statistics variable is not possible.
- A formula contains the sample identification 3 (C23). The variable has been replaced by -0.
- The method contains the parameter 'activation pulse: first'. This parameter has been ignored.
- Measuring input 'diff.' has been replaced by measuring input '1'.
- The relative start volume has been replaced by 0.00 mL.
- The relative stop volume has been replaced by 100.00 mL.
- SET: The delay time for EP1 and EP2 was set to 'inf.'
- The method contains the evaluation 'fix time'. This parameter is ignored.
- An old method file with the same name has been replaced.
- The method file has been renamed to: New method name

Conversion not possible (red-marked methods)

- The method could not be converted.
- This mode is not supported. Only DET, MET, SET, KFT, STAT, MEAS and DOS can be converted.
- Conditioning is switched on. The method cannot be converted.
- This mode is not supported. Only STAT pH/U can be converted.
- The measured quantity Ipol/Upol being monitored is not supported. Check the monitoring settings.

6.8 Arithmetic algorithms in the Titrand

Some of the algorithms and number formats used in the instrument software are explained subsequently.

Number format

The standard IEEE 754 (1985) for binary floating-point arithmetic has been implemented in the software as "single precision" (32 Bit).

Rounding method

Measured values and results are displayed rounded, depending on user settings. For that purpose, arithmetic rounding is carried out according to the following method:

Example for rounding to $n = 3$ decimal places:

1. $99.644499 \xrightarrow{\cdot 10^n} 99644.499$
2. $99644.499 \xrightarrow{+ 0.5} 99644.999$
3. $99644.999 \xrightarrow{\text{cut}} 99644$
4. $99644 \xrightarrow{\cdot 10^{-n}} 99.644$

Statistics

The arithmetic mean value as well as the absolute and relative standard deviation are calculated for results R, endpoints EP and variables C:

A maximum of nine results with 20 determinations each at the most can be evaluated statistically out of a determination.

The following convention applies to the subsequent formulas:

$$1 \leq n \leq 20$$

$$1 \leq k \leq 9$$

Mean value \bar{x}_k :

$$\bar{x}_k = \frac{1}{n} \cdot \sum_{i=1}^n R_{k,i}$$

Absolute standard deviation S_{abs_k} :

$$S_{abs_k} = + \sqrt{\frac{\sum_{i=1}^n (R_{k,i} - \bar{x}_k)^2}{n-1}}$$

Relative standard deviation S_{rel_k} (in %):

$$S_{rel_k} = 100 \cdot \frac{S_{abs_k}}{\bar{x}_k}$$

Explanation

The statistical calculations in the software have been implemented in such a way that they are as revisable as possible for the user. This is why the individual values used in the statistics are in the rounded presentation form selected by the user.

It is not the number of decimal places which is decisive for the accuracy of the calculations, but rather the number of significant digits of the decimal numbers displayed. As a result of the binary 32-bit number format implemented on the basis of the IEEE 754 standard, the decimal numbers which are produced have 7 reliable significant decimal digits.

You can influence the number of significant digits by selecting the unit and the number of decimal places. As the results unit to be set sometimes contains both the prefix "milli" and the physical unit itself, the number of significant digits is altered accordingly in such a case by three digits.

Example:

The displayed result 1234,56789 mg/L has 7 reliable digits. It is to be rounded to three decimal places according to the rounding method given above:

1234,568 mg/L	(7 significant digits, 3 of which are decimal places)
---------------	---

With the unit "g/L" the same result 1.23456789 g/L is also rounded to three decimal places:

1.235 g/L	(4 significant digits, 3 of which are decimal places)
-----------	---

The number of significant digits has now been reduced by three to four digits by omitting the prefix "milli".

You will obtain the smallest loss of rounding accuracy by selecting the application and number format so that the displayed numbers contain as many pre-decimal places as possible.

A complete recalculation of the statistics using a pocket calculator or a PC calculation program can produce variations. This is caused by the different binary number formats used in these instruments. Whereas the Titrand calculate with binary 32-bit numbers as described above, PC programs (e. g. MS-Excel) use a different binary format, e. g. IEEE 754 64-bit.



Note!

The losses of accuracy by rounding described above in the range of the maximum reliable digits are only of theoretical relevance. Most of the time they are lower by several orders of magnitude than – as an example – the uncertainties resulting from weighing out the sample.

6.9 Standard equipment

Immediately upon receipt of the Touch Control or PC Control software please check that the delivery is complete. Please also consult the lists of accessories in the Installation Instructions for the Titrando, where the Titrando accessories are described.

6.9.1 840 Touch Control

No.	Order no.	Description
1	1.840.0100	840 Touch Control
1	6.6051.000	CompactFlash card with user methods and 6.2247.000 Adapter
1	A.704.0007	PC Control CD-ROM
1	8.840.8003EN	Manual PC Control / Touch Control
1	8.840.1413	Tutorial Touch Control

6.9.2 PC Control software with Dongle (6.6050.400)

No.	Order no.	Description
1	A.704.0007	PC Control CD-ROM
1	6.2145.100	USB dongle
1	8.840.8002EN	Installation PC Control
1	8.840.8003EN	Manual PC Control / Touch Control
1	8.840.1513	Tutorial PC Control

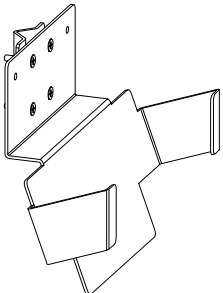
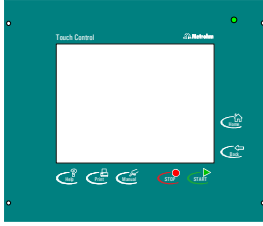
6.9.3 PC Control software, demo version (6.6050.405)

The demo version is fully functional for 100 days after installation. After this period has elapsed you must purchase a USB dongle.

No.	Order no.	Description
1	A.704.0007	PC Control CD-ROM
1	8.840.8002EN	Installation PC Control
1	8.840.8003EN	Manual PC Control / Touch Control
1	8.840.1513	Tutorial PC Control

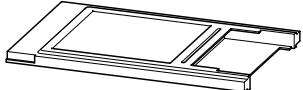
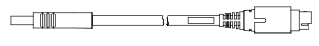
6.10 Additional devices and optional accessories

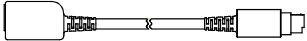
6.10.1 Miscellaneous accessories

Order no.	Description	
6.2145.100	USB dongle	
6.2162.000	Bluetooth USB adapter for Touch Control 840	
6.2051.030	Wall holder for attaching the Touch Control to a wall or support rod (diameter 10 mm). You can also use the wall holder to achieve a steeper display angle on the bench.	
6.2834.030	Spare film for 840 Touch Control 3 pieces The films can be exchanged when they become dirty or damaged.	
6.2133.010	Batteries 1.5 V, 2 pieces Spare batteries for Touch Control, 1.5 V LR6	

6.10.2 Communication

Further cables can be found in the Installation Instructions for the Titrandos.

Order no.	Description	
6.2247.000	Adapter CompactFlash card – PC card type II Adapter for using CompactFlash cards in PCMCIA card slots	
6.2247.010	CompactFlash card 32 MB Memory card for methods, determinations, sample data silos, etc.	
6.2151.000	Cable for connecting a Titrandos to a PC (USB connection, type A) and for connecting further Titrandos USB A – Controller (1.8 m)	

<i>Order no.</i>	<i>Description</i>
6.2151.010	Extension cable for MSB connections and for Touch Control – Titrande mini-DIN socket – mini-DIN plug (2 m) 

6.11 Warranty and conformity

6.11.1 Warranty

Metrohm guarantees that the deliveries and services it provides are free from material, design or manufacturing errors. The warranty period is 36 months from the day of delivery; for day and night operation it is 18 months. The warranty remains valid on condition that the service is provided by an authorized Metrohm service organization.

Glass breakage is excluded from the warranty for electrodes and other glassware. The warranty for the accuracy corresponds to the technical specifications given in this manual. For components from third parties that make up a considerable part of our instrument, the manufacturer's warranty provisions apply. Warranty claims cannot be pursued if the Customer has not complied with the obligations to make payment on time.

During the warranty period Metrohm undertakes, at its own choice, to either repair at its own premises, free of charge, any instruments that can be shown to be faulty or to replace them. Transport costs are to the Customer's account.

Faults arising from circumstances that are not the responsibility of Metrohm, such as improper storage or improper use, etc. are expressly excluded from the warranty.

6.11.2 Declaration of Conformity

Software Validation

 **Metrohm**
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CH-9101 Herisau, Switzerland
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Fax +41 71 353 89 01
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for the program

PC Control 5.0

Description

PC software for controlling Metrohm titration and automation instruments. Simple and intuitive user guidance. Creation of methods, carrying out titrations, storage and recalculation of results. Methods and data are compatible with Touch Control. Contains numerous tried and tested titration methods. Including hardware Dongle. Dialog in English, German and further freely definable languages.

6.6050.400 PC Control 5.0 Software

The software mentioned above was developed in accordance with the requirements of the ISO 9001 quality system regarding the design, testing and servicing of Metrodata software. The relevant procedures are described in the attached document "Project procedure for creating Metrodata software".

The technical specifications are documented in the installation manual.

The software was validated with respect to functionality, analytical performance and accuracy of results. The software functions are documented in the manual.

Herisau, 22 May, 2008







D. Strohm
Vice President
Head of R&D



A. Dellenbach
Head of Quality Management

6.11.3 Declaration of Conformity

This is to certify the conformity to the standard specifications for electrical appliances and accessories, as well as to the standard specifications for security and to system validation issued by the manufacturing company.

<p><i>Name of commodity</i></p> <p>840 Touch Control</p>	 CH-9101 Herisau/Switzerland E-Mail info@metrohm.com www.metrohm.com
<p><i>Description</i> Control unit with touch-sensitive screen for Metrohm titration and automation instruments and peripheral devices such as dosing devices, stirrers and titration stands.</p>	
<p>This instrument has been built and has undergone final type testing according to the standards:</p> <p><i>Electromagnetic compatibility: Emission</i> EN/IEC 61326-1: 2006, EN/IEC 61000-6-3: 2001, EN 55022 / CISPR 22: 2003</p> <p><i>Electromagnetic compatibility: Immunity</i> EN/IEC 61326-1: 2006, EN/IEC 61000-6-2: 2005, EN/IEC 61000-4-2: 2001, EN/IEC 61000-4-3: 2002</p> <p><i>Safety specifications</i> EN/IEC 61010-1: 2001, UL 61010-1: 2004, CSA-C22.2 No. 61010-1: 2004, protection class III</p> <p>It has also been certified by ElectroSuisse, which is member of the International Certification Body (CB/IEC).</p>	
<p> <i>This instrument meets the requirements of the CE mark as contained in the EU directives 2006/95/EC (LVD), 2004/108/EC (EMC). It fulfils the following specifications:</i></p> <p>EN 61326-1 Electrical equipment for measurement, control and laboratory use – EMC requirements</p> <p>EN 61010-1 Safety requirements for electrical equipment for measurement, control and laboratory use</p>	
<p>Metrohm Ltd. is holder of the SQS certificate ISO 9001:2000 Quality management system for development, production and sales of instruments and accessories for ion analysis.</p>	
<p>The system software, stored in Read Only Memories (ROMs) has been validated in connection with standard operating procedures in respect to functionality and performance.</p> <p>The technical specifications are documented in the manual.</p>	
<p>Herisau, 22 May, 2008</p> <div style="display: flex; justify-content: space-around; align-items: flex-end;"> <div style="text-align: center;">  D. Strohm Vice President Head of R&D </div> <div style="text-align: center;">  A. Dellenbach Head of Quality Management </div> </div>	

6.11.4 Quality Management Principles

Metrohm Ltd., CH-9101 Herisau, Switzerland

**Metrohm**
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Metrohm Ltd. holds the ISO 9001 Certificate, registration number 10872-02, issued by SQS (Swiss Association for Quality and Management Systems). Internal and external audits are carried out periodically to assure that the standards defined by Metrohm's QM Manual are maintained.

The steps involved in the design, manufacture and servicing of instruments are fully documented and the resulting reports are archived for ten years. The development of software for PCs and instruments is also duly documented and the documents and source codes are archived. Both remain the possession of Metrohm. A non-disclosure agreement may be asked to be provided by those requiring access to them.

The implementation of the ISO 9001 quality system is described in Metrohm's QM Manual, which comprises detailed instructions on the following fields of activity:

Instrument development

The organization of the instrument design, its planning and the intermediate controls are fully documented and traceable. Laboratory testing accompanies all phases of instrument development.

Software development

Software development occurs in terms of the software life cycle. Tests are performed to detect programming errors and to assess the program's functionality in a laboratory environment.

Components

All components used in the Metrohm instruments have to satisfy the quality standards that are defined and implemented for our products. Suppliers of components are audited by Metrohm as the need arises.

Manufacture

The measures put into practice in the production of our instruments guarantee a constant quality standard. Production planning and manufacturing procedures, maintenance of production means and testing of components, intermediate and finished products are prescribed.

Customer support and service

Customer support involves all phases of instrument acquisition and use by the customer, i.e. consulting to define the adequate equipment for the analytical problem at hand, delivery of the equipment, user manuals, training, after-sales service and processing of customer complaints. The Metrohm service organization is equipped to support customers in implementing standards such as GLP, GMP, ISO 900X, in performing Operational Qualification and Performance Verification of the system components or in carrying out the System Validation for the quantitative determination of a substance in a given matrix.

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