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PC Control

**For controlling
Titrandos**

Tutorial

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Although all the information given in the tutorial has been checked with great care, errors cannot be entirely excluded. Should you notice any mistakes please inform the author at the address given above.

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1 Introduction

This tutorial describes how to control a Titrande with the PC Control software. It is intended to introduce you to the operating elements and working steps that are necessary to carry out an automatic titration.

The course is divided into four sections:

- **Section 1: Introduction**

First you will learn the most important steps for the configuration of your titration system.

- **Section 2: Acid/Base titration**

You load a method, start the titration and have the result displayed.

- **Section 3: Titration with further functions**

In this section you will learn how to create your own method and to calculate statistics covering several titrations. In addition you will learn how you can simplify the processing of large series of samples by using the sample data silo.

- **Section 4: Tips**

Further information concerning the use of the Titrande system is briefly described. In section 2 and section 3 you will find references (→**TIP**) for these tips.

Detailed information about the operation of the Titrande system can be found in the online help and in the corresponding Instructions for Use:

- Installation Instructions for Titrande
- Instructions for Use for PC Control / Touch Control
- Instructions for Use for 806 Exchange Unit
- Instructions for Use for 800 Dosino or 807 Dosing Unit

1.1 Requirements

1.1.1 Equipment

The following instruments, accessories and solutions are required for the titration described below:

- **Titrand** (*with* internal dosing drive) with **806 Exchange Unit** or **Titrand** (*without* internal dosing drive) with **800 Dosino** and **807 Dosing Unit**
- Computer with **PC Control software**
- **801 Magnetic Stirrer** or **803 Ti Stand** or **804 Ti Stand** with **802 Rod stirrer**
- **Titrand** $c(\text{NaOH}) = 0.1 \text{ mol/L}$ (carbonate-free)
- **Sample** $c(\text{HCl}) = 0.1 \text{ mol/L}$
- Distilled water (CO_2 -free if possible)

1.1.2 Installation

Before you start this course you must ensure that the whole titration system has been correctly installed. Details can be found in the **Installation Instructions** for the Titrand. The installation of the PC Control software is described in the **Instruction for Use** for PC Control / Touch Control.

The most important points for the installation of the instruments are given briefly below in sequence:

1. Connect the computer
2. Connect the stirrer
3. Connect the dongle
4. Connect the Dosino (if present)
5. Attach the exchange/dosing unit
6. Connect the pH electrode
7. Connect to the mains supply

Please note that in the following exemplary methods the stirrer is connected to **MSB 1** of the Titrand. This means that if a Titrand without internal dosing drive is used then the external dosing device (in this case Dosino) must be connected to the MSB connection of the stirrer. In this way it will be addressed as **Dosing device 1**, like an internal dosing drive of a Titrand.

1.2 Preparations

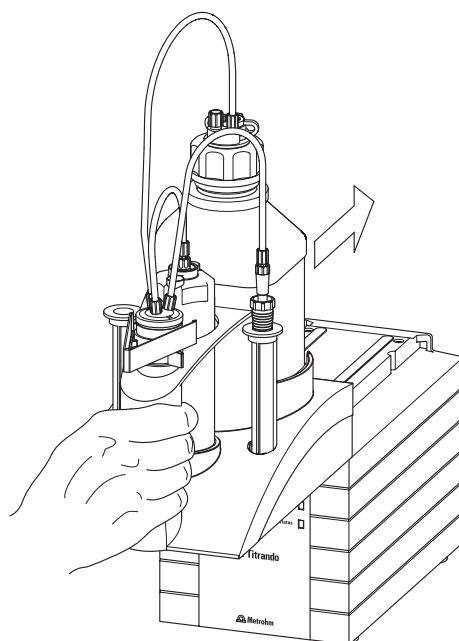
1 Equip the exchange unit or Dosino with titrant

In this example 0.1 M NaOH is used as the titrant. Depending on the system setup, equip the 806 Exchange Unit or the 807 Dosing Unit with a suitable bottle containing this solution. A detailed description is given in the Instructions for Use of the exchange unit or dosing unit.

2 Attach the exchange unit (Titrande with internal dosing drive)

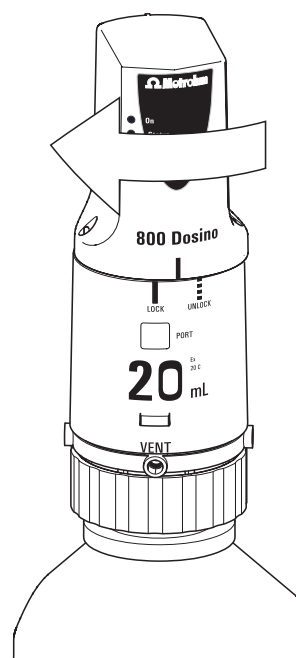
Attach the exchange unit to the Titrande.

Slide it onto the guide rail of the Titrande from the front and push it back so that it snaps into position:



Attach the Dosino to the dosing unit (Titrande without internal dosing drive)

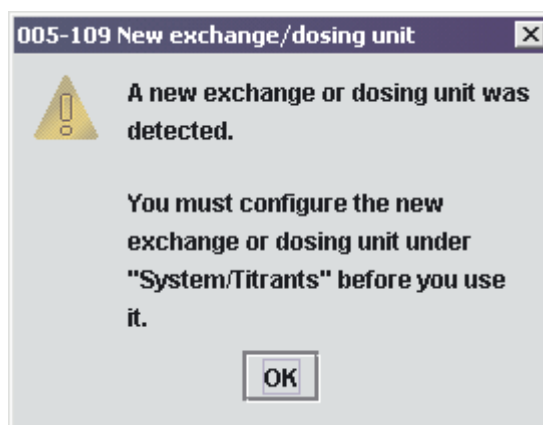
Attach the Dosino to the dosing unit mounted on the titrant bottle. Please observe the markings provided on the Dosino and on the dosing unit (see also 800 Dosino Instructions for Use).



3 Start PC Control

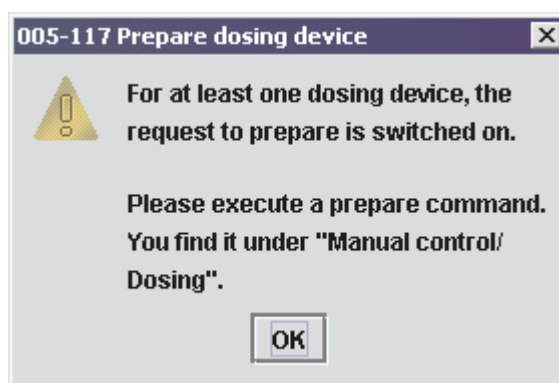
Start the **PC Control** program on your computer.

If you use a new exchange or dosing unit which has not yet been configured, the program will then produce the following message:



The configuration of the new exchange or dosing unit is described in step **7**.

Next you will also be requested to carry out the "Prep" function in order to rinse all the tubing:

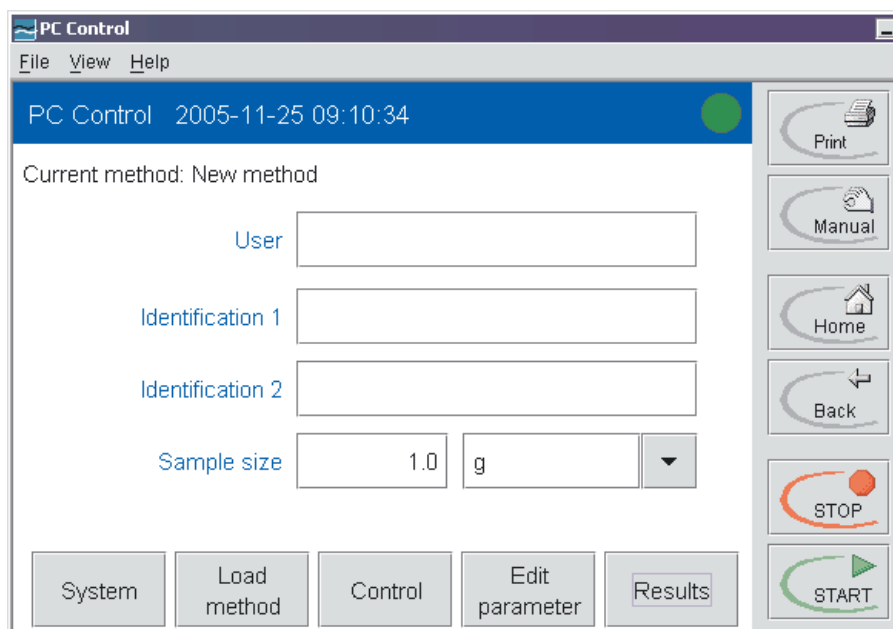


The preparation of the dosing device is described in step **8**.

If the data chip of the exchange or dosing unit already contains titrant data then you will be asked whether these data are to be transferred to the list of titrants (Message: 005-110 New titrant). This should be answered with [Yes] so that the titrant data are copied to the PC Control titrant list. Changes are stored on the data chip.

4 Main dialog

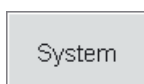
After initialization has been carried out this program window is displayed:



The PC Control desktop contains the following operating elements, which can be activated by a mouse click:



Fixed keys [Print], [Manual], [Home], [Back], [STOP], [START] provide a function which is independent from the dialog content. They can be activated at any time.



Buttons are used to open a new dialog page or to trigger certain functions.



Input fields are used to edit numbers and text.



Button to open a selection list.

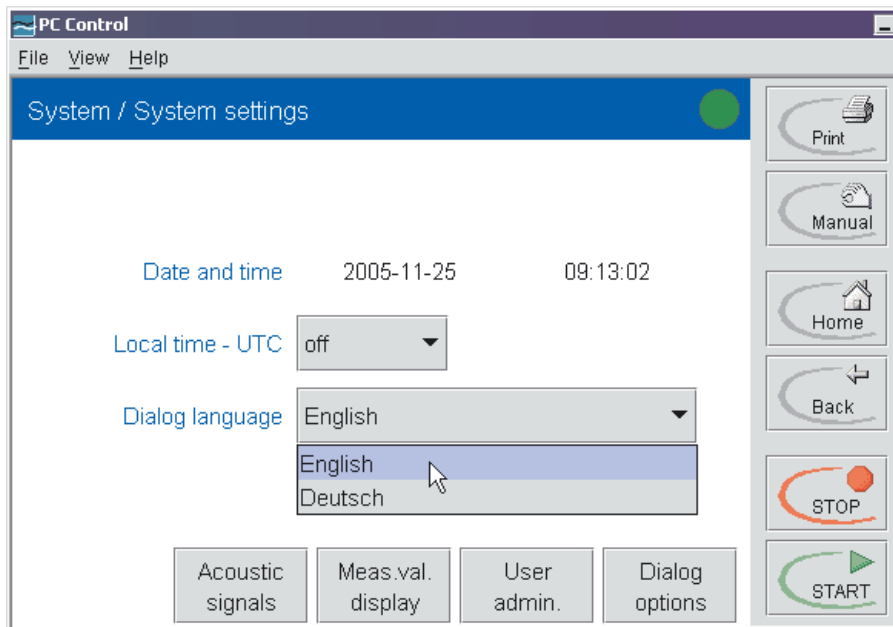
5 Check date and time

In the blue status line the current date and time are shown.

If these are not correct then you should correct them in the system settings of the operating system. If necessary, contact the responsible system administrator.

6 Change the dialog language

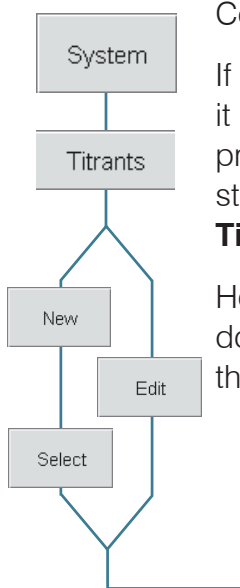
To change the dialog language, click on the [System] button in the main dialog and then [System settings] in the following selection. Open the selection list for **Dialog language** with a mouse click:



Select the new dialog language. The procedure to load a new dialog language is described in the Instructions for Use for PC Control / Touch Control.

Return to the main dialog with the fixed key [Home].

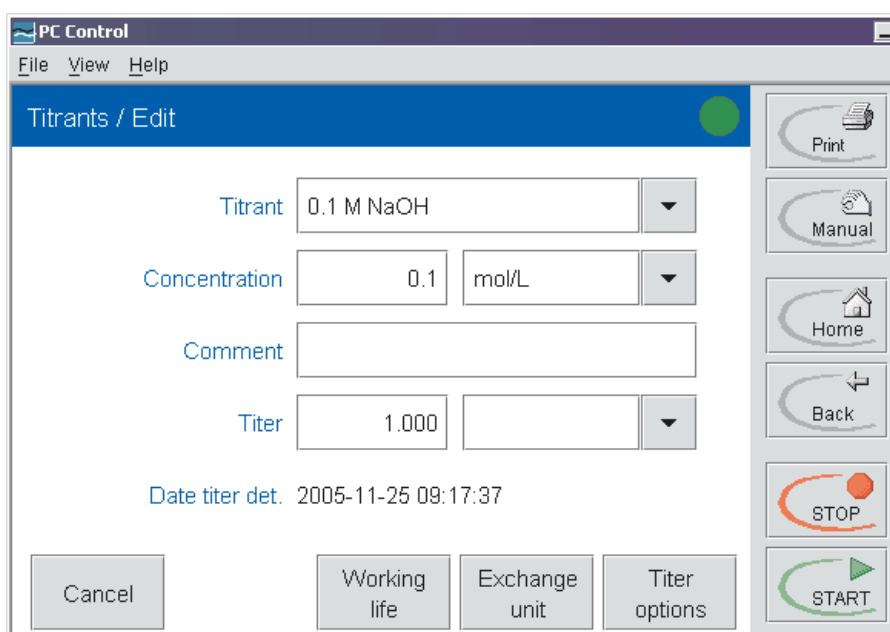
7 Configure a new titrant



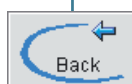
Configure the new titrant under **System / Titrants**.

If the exchange or dosing unit has not yet been used (see step **3** then it will not be shown here. In this case click on [New], after which the program will show the connected **Dosing device 1 (D1)** on the instrument **Titrand 1**. Select this with [Select]. This enters the dialog **Titrants / Edit**.

However, if you already find a titrant with an intelligent exchange or dosing unit (IEU or IDU) on **Dosing device 1** under **System / Titrants** then this can be modified with [Edit]:



Here you can name the **Titrant** as being **0.1 M NaOH**. In the **Concentration** field enter the titrant concentration in mol/L: **0.1**. Please observe the country-specific settings on your computer for writing the decimal separator. If you know the titer of the sodium hydroxide used then you can also enter it here, as it will be used for calculation in a later step.



With a click on [Back] you will return to the list of titrants:

Titrant	Cyl.	Type	Dos.device
0.1 M NaOH	20 mL	IEU	D1

You now have an intelligent exchange unit (IEU) or dosing unit (IDU) available at dosing device 1 with the titrant 0.1 M NaOH. In this example the cylinder volume is 20 mL, but may be different in your system.



You can return to the main dialog with [Home].

8 Prepare the dosing device

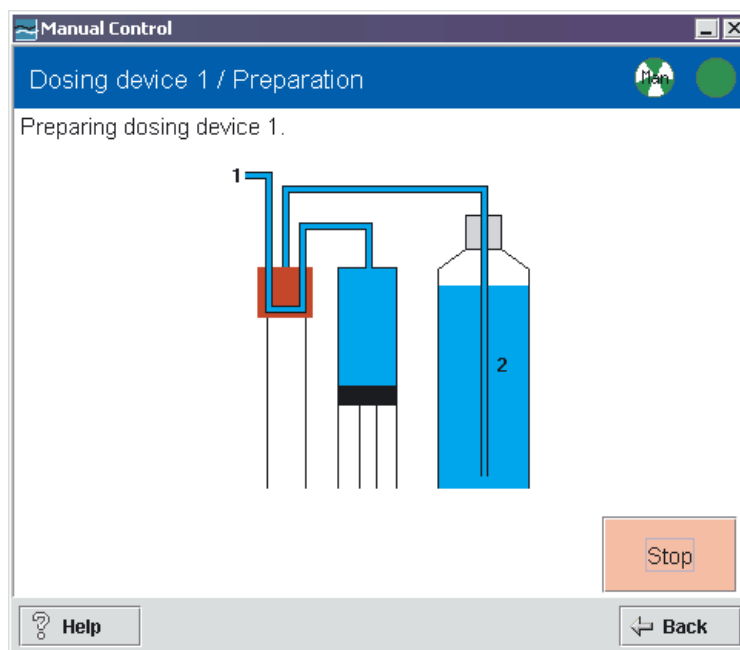
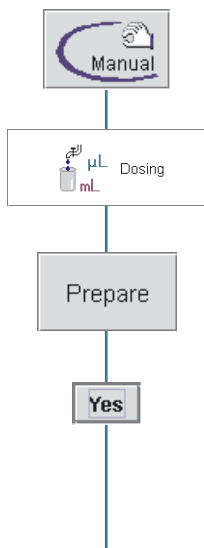
The cylinder and all the tubing connections of the dosing device must be rinsed and filled with titrant.


This is done by using the fixed key [Manual] to start **Manual operation**. Now click on [Dosing].

The most important titrant data are shown; click on [Prepare].

The **Splash warning** which now appears informs you that the buret tip of the dosing device should be pointed into a vessel which can accommodate several cylinder volumes.

After this message has been confirmed with [Yes] the dosing cylinder will be emptied and refilled twice. The animation shown makes this process clear; here it is shown for an exchange unit:



Please also note the animated symbol "Manual Busy" , which shows you both here and in the main dialog that manual operation is active. It disappears as soon as the process has been completed.

Close the **Manual Control** window with a click on the "X" in the top right-hand corner.

Your Titrand system is now properly set up and ready to carry out an automatic titration!



2 Acid/Base titration

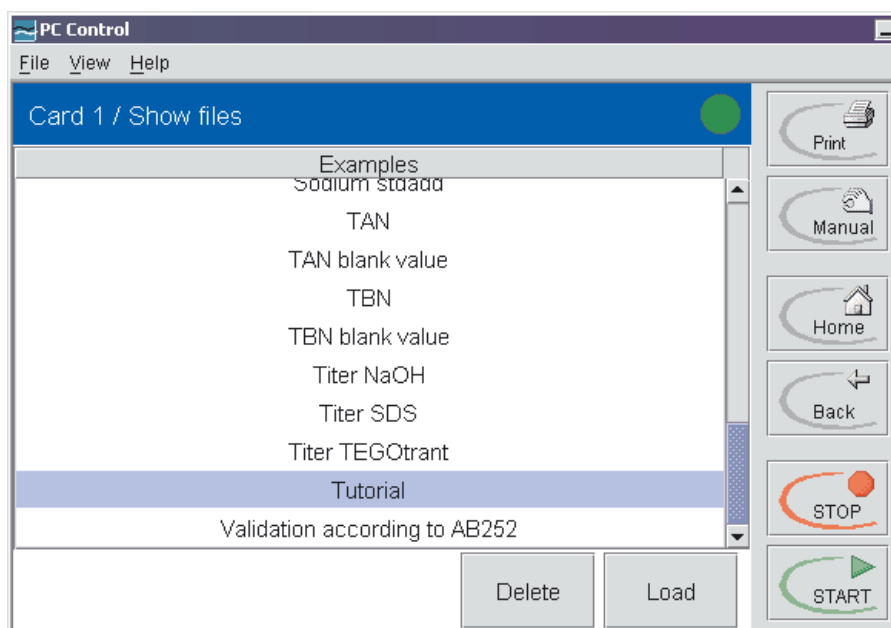
The following example of a simple titration of hydrochloric acid with sodium hydroxide assumes that you are using a 20 mL exchange unit or dosing unit, but all other exchange or dosing units can also be used.

1 Load method

Load method

Card 1

In the main dialog click on [Load method]. Then choose [Card 1] and select the method **Tutorial** in the group **Examples**:



Load

Click on [Load].

In the main dialog "**Tutorial**" will now be displayed as the current method.

2 Add hydrochloric acid

➔ **TIP 1**

Place 50 mL dist. H₂O and 5 mL 0.1 M hydrochloric acid in a 100 mL beaker. Then immerse the pH electrode and the dosing tip into the solution.

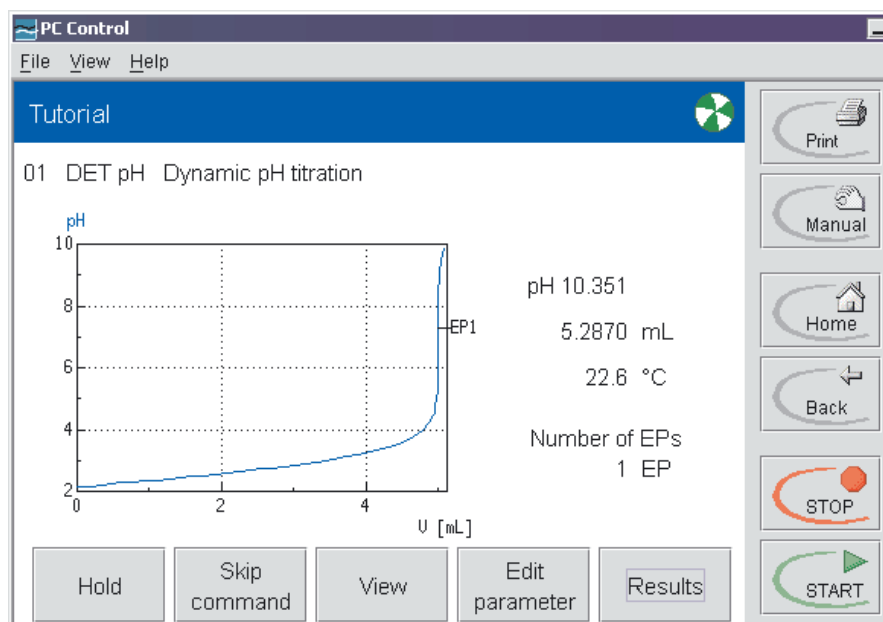
Enter the **Sample size** (5 mL) in the main dialog:

Sample size mL

3 Start the titration

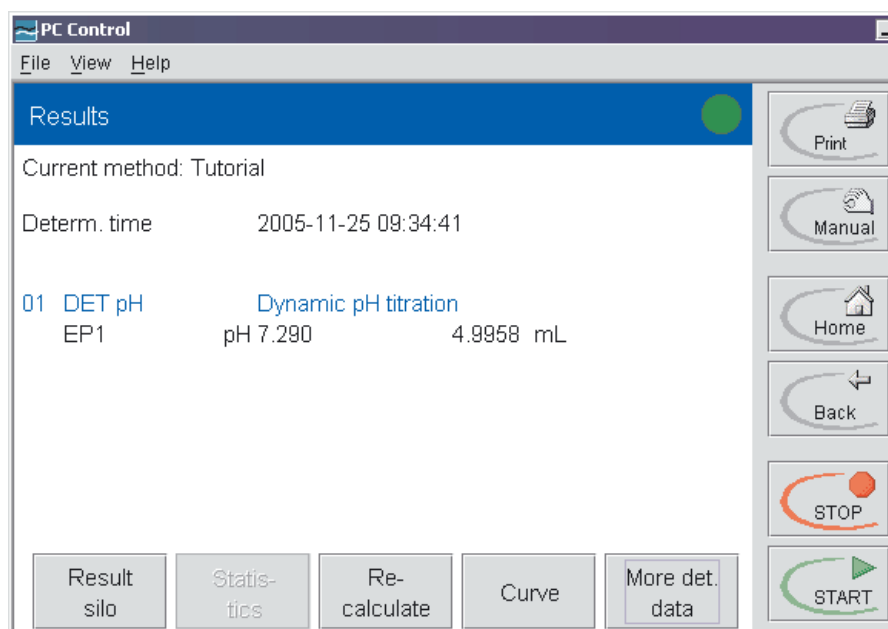


In the main dialog click on [START]. The titration starts with the measurement of the initial measured value. After this the running titration is shown in the live display:



4 Result display

When the endpoint has been reached the result will be shown:



The volume of the added NaOH is given directly as the result. Depending on the CO₂ content of the H₂O(dist.) or the NaOH used an additional equivalence point EP2 may also be detected.

→ TIP 2

To view the titration curve click on [Curve]. You can return to the main dialog with [Home].

3 Titration with additional functions

Now that you have successfully carried out a simple acid/base titration this section will familiarize you with some of the important options of the Titrand system. You will first create your own method using a method template and then carry out the titration by using various options.

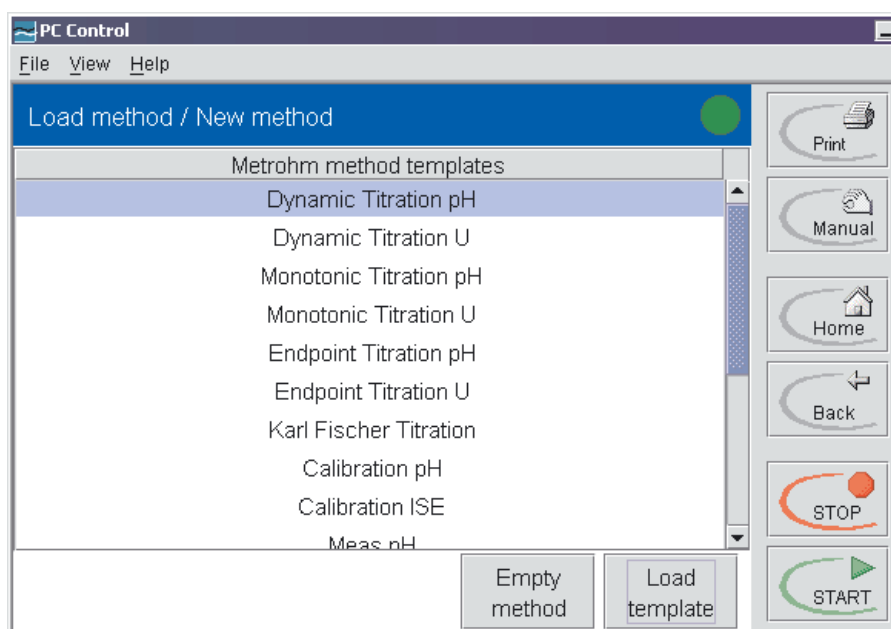
3.1 Creating methods

1 Create a new method

Load method

New method

The easiest way of creating a new method is by modifying a **Method template**. This template is selected under **Load method / New method**:



Load template

Select the **Dynamic Titration pH** template and then click on [Load template].

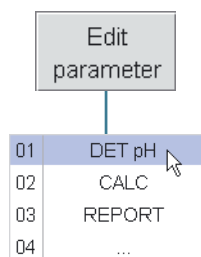
Edit parameter

You have loaded the basic structure of a method for pH titration with dynamic titrant addition, whose commands can be viewed and modified with [Edit parameter]:

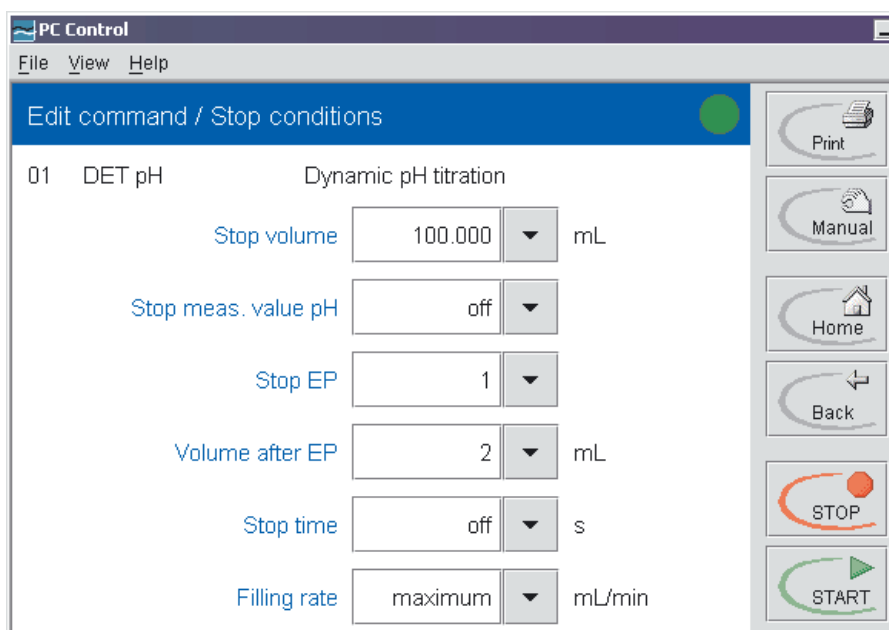
01	DET pH	Dynamic pH titration
02	CALC	Calculation
03	REPORT	Report
04	...	

Individual parameters must still be edited.

2 Edit method parameters



01 DET pH / Stop conditions: as the previous titration this titration is also to be ended as soon as the first equivalence point has been detected (**Stop EP: 1**). Then a further 2 mL titrant is to be added in order to obtain a symmetrical curve (**Volume after EP: 2 mL**). Edit these parameters accordingly. The stop volume should be retained for safety reasons or adapted to suit the volume of the titration vessel.



PC Control
File View Help

Edit command / Stop conditions

01 DET pH Dynamic pH titration

Stop volume 100.000 mL

Stop meas. value pH off

Stop EP 1

Volume after EP 2 mL

Stop time off s

Filling rate maximum mL/min

Print

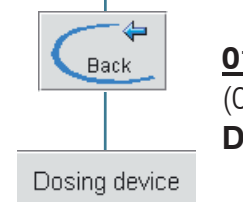
Manual

Home

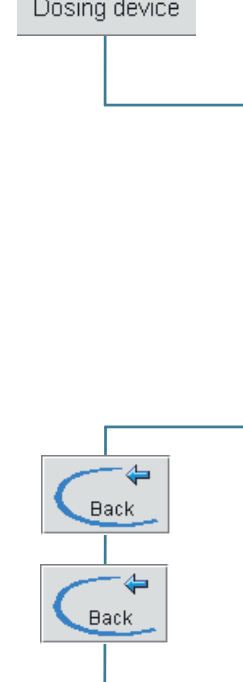
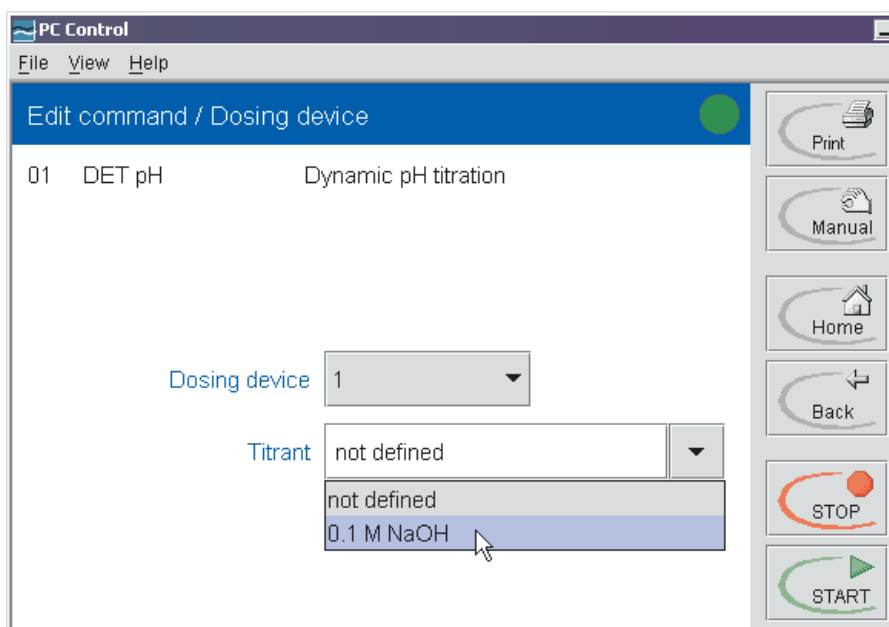
Back

STOP

START



01 DET pH / Dosing device: the next step is to define the titrant (0.1 M NaOH) under **Edit parameter / Edit command (01 DET pH) / Dosing device:**

PC Control
File View Help

Edit command / Dosing device

01 DET pH Dynamic pH titration

Dosing device 1

Titrant not defined

not defined

0.1 M NaOH

Print

Manual

Home

Back

STOP

START

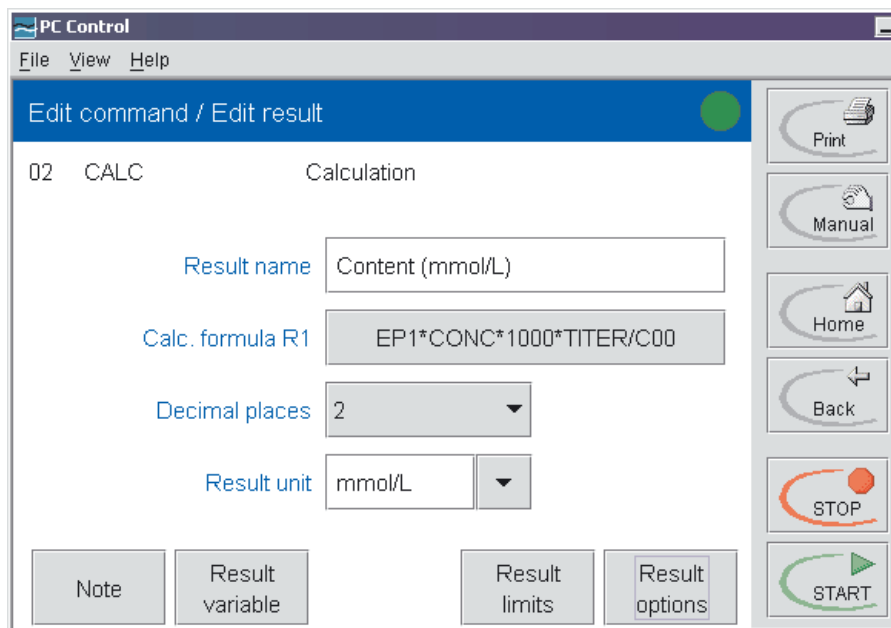
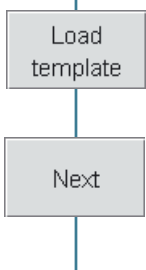
01	DET pH
02	CALC
03	REPORT
04	...

02 CALC: in this method sequence a result is to be calculated after the titration. The corresponding command **CALC** is already inserted in the template, but does not yet contain a calculation. Select **CALC** in line 2 and create a new result calculation with [Edit command] and [New] as follows:



Select the template **Content (mmol/L)**, load this with [Load template] and click on [Next]. The result calculation that appears can be used directly. It uses the volume of the first equivalence point (EP1) to determine the content of hydrochloric acid in mmol/L.

- Metrohm result templates
- Content (g/L)
- Content (mmol/L)
- Content (mol/L)



The result R1 is calculated from the following quantities:

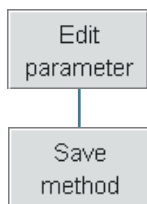
- EP1:** Volume of the titrant at equivalence point 1 [mL]
- Conc:** Concentration of the titrant [mol/L]
- 1000:** Factor to convert the concentration from mol/L to mmol/L
- TITER:** Titer of titrant
- C00:** Sample size [mL]

→ TIP 3

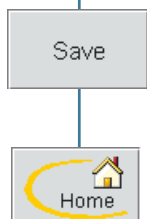
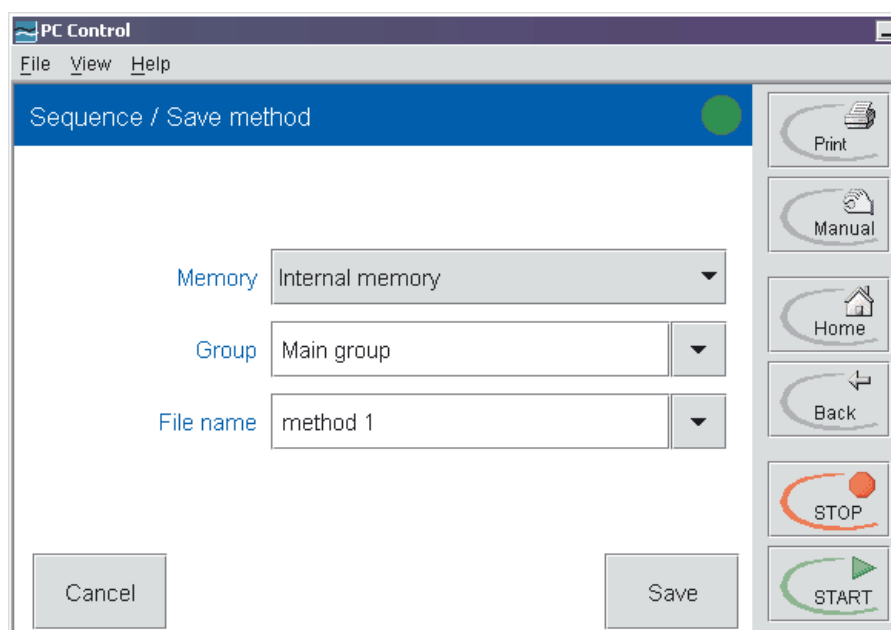
The **sample size** is entered in the corresponding field in the main dialog before the start of the titration. You can also define an automatic request for this value with a REQUEST command or its transfer from a connected balance at the start of a method sequence (see Instructions for Use for PC Control / Touch Control).

03 Report: the third command in the method sequence describes the report output on the printer selected in the menu **File / Printer**. In this example the result report and the titration curve are printed out. The report command does not need to be altered. Delete this command if no printer is connected to your PC.

3 Save new method



The new method is saved under **Edit parameter / Save method**:



In this example the method is saved as **method 1** in the group **Main group** in the **Internal memory**.

With a mouse click on the input field, you edit the group name or the file name.

Confirm the entry with [Save] and return to the main dialog with [Home].

→ TIP 4

3.2 Titrating

1 Carrying out a titration

→ TIP 1

Prepare the electrode and the titration vessel for a new determination and carry out the titration as described in Section 2.

As the method sequence contains an automatic report printout on the connected printer please ensure that the connection is functioning.

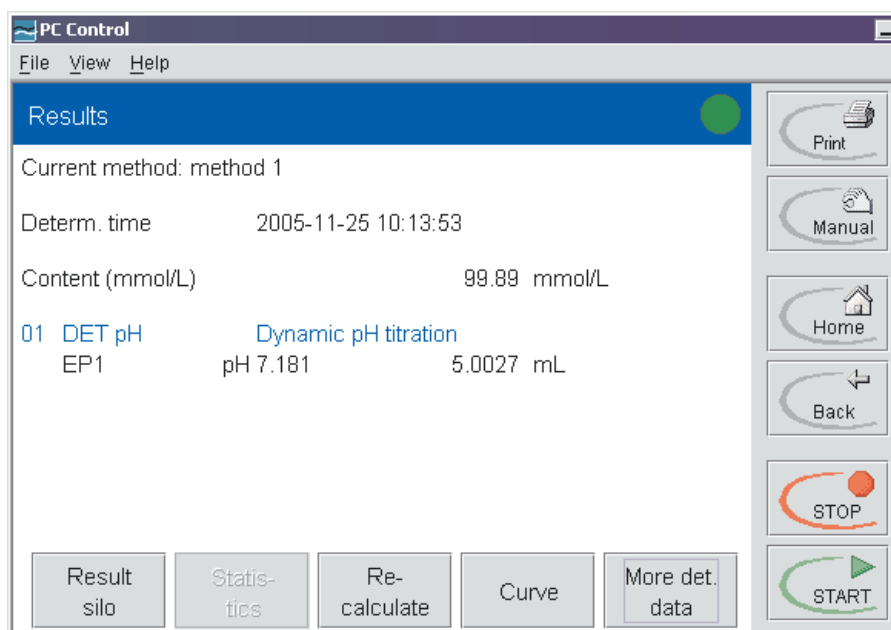
Enter the sample size (5 mL) in the main dialog.



Start the titration with [START].

2 Result display

When the endpoint has been reached the result will be shown:



The calculated content of the hydrochloric acid is shown as the result. To show the titration curve click on [Curve]. You can return to the main dialog with [Home].

→ TIP 5

3 Report output

The report output supplies the following printout:

PC Control PC Control	Serial number 3079972211 Printed	Program version 4.0 2005-11-25 10:15:38
Result report		
Determination	Method method 1 Last saved on 2005-11-25 10:05:02 ver. 1 Method status saved Determin. time 2005-11-25 10:13:53 Status of deter. original Sample number 1	
Sample data	Sample size 5 mL	
01 DET pH	Dynamic pH titration	
Titration	EP1 pH 7.181 5.0027 mL Stop EP reached	
Results	Content (mmol/L) 99.89 mmol/L	
Curve		
01 DET pH	Dynamic pH titration	
<p>The graph displays a titration curve for a dynamic pH titration. The vertical axis represents pH, ranging from 2 to 12 with major ticks every 2 units. The horizontal axis represents Volume (V [mL]), ranging from 0 to 6 with major ticks every 2 units. The curve starts at a pH of approximately 2.2 at 0 mL and remains relatively flat until about 4 mL. Between 4 mL and 5 mL, there is a sharp, nearly vertical increase in pH, reaching a plateau of approximately 11.5. A point on the curve is labeled 'EP1' at approximately 5.0027 mL and pH 7.181. Dotted grid lines are present for both axes.</p>		

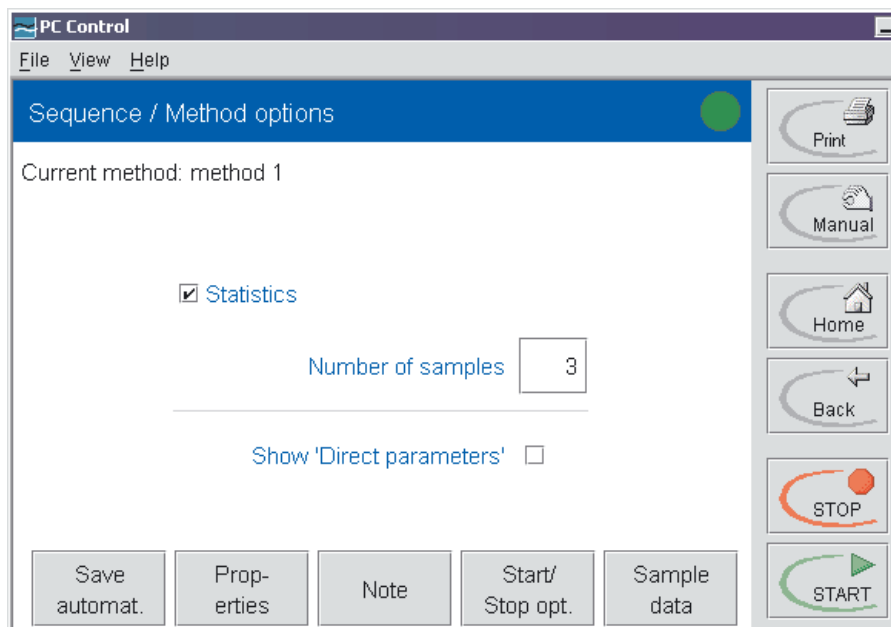
3.3 Statistics and sample data silo

1 Prepare statistics

For a statistical evaluation of several results activate the statistics under **Edit parameter / Method options**:

Edit parameter

Method options



Enter the number of samples to be investigated (in this case "3").

You do not need to return to the main dialog every time with [Back] or [Home] in order to start a determination. Start the following titration directly from here with [START].

2 Carrying out titrations for statistics

Prepare the electrode and the titration vessel for a new determination and carry out three titrations as described in Section 2. Enter a sample identification and the sample size in the main dialog before each titration.

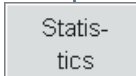
After each titration a report will be printed out and the result shown. On the main dialog you can see how the determinations are counted for the statistics:



3 x

Statistics: 1 of 3

After the third titration click on [Statistics] in the result display.

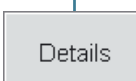


The name of the result and its mean value will be shown at first:

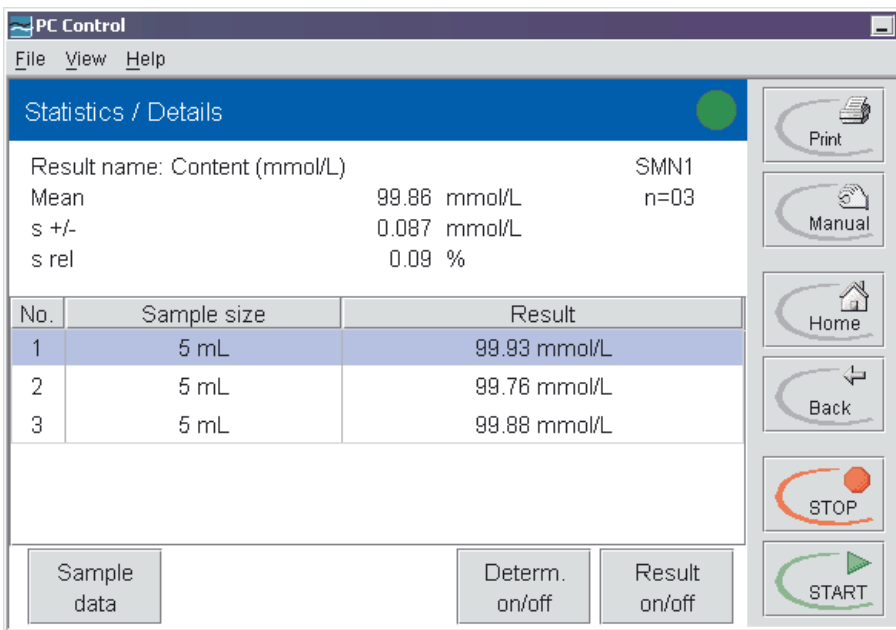
Current method: method 1
Determinations 3 of 3

Result name	Mean
Content (mmol/L)	99.86 mmol/L

Now click on [Details].



Further statistical data and the individual results will be shown:



The screenshot shows the 'PC Control' software interface. The title bar reads 'PC Control' and the menu bar has 'File View Help'. The main window title is 'Statistics / Details'. The screen displays the following information:

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 mL	99.93 mmol/L
2	5 mL	99.76 mmol/L
3	5 mL	99.88 mmol/L

At the bottom of the window, there are three buttons: 'Sample data', 'Determ. on/off', and 'Result on/off'. On the right side, there is a vertical toolbar with buttons for 'Print', 'Manual', 'Home', 'Back', 'STOP', and 'START'.

3 Print statistics



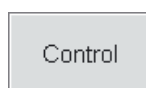
If you like to produce a report containing these statistics then click on [Print]. The context-sensitive function of this key allows the direct selection of a statistics report.

Statistics overview

Click on **Statistics overview**, for example.

A report containing all the statistical data and individual results will now be printed out.

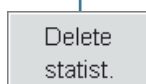
4 Sample data silo



Prepare a **sample data silo** for a series of determinations.

Sample data silo

Activate sample data silo: activate the sample data silo in the main dialog under **Control**. Delete all the statistics data with [Delete statistics].



Then click on [Sample data silo] in the main dialog. The sample data silo will now be shown below the program window. Initially it does not contain any sample data. Enter these as described below.



Sample data silo

The screenshot shows the PC Control software interface. At the top, it displays 'PC Control 2005-11-25 11:39:58'. Below this, it shows 'Current method: method 1' and a 'User' input field. The 'Sample data silo' section is active, showing 'Line 0 of 3' and a 'Sample data silo' button. Below that, it shows 'Statistics: 0 of 3'. At the bottom, there is a table with the following data:

No.	Method	Identification 1	Identification 2	Smpl size	Unit
> 1		sample 1		5 mL	
2		sample 2		5 mL	
3		sample 3		5 mL	

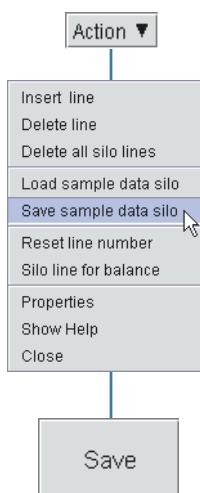
Enter sample data: for the samples you should enter e. g. a sample identification and the sample size unit "mL". Activate the particular input field with a mouse click and change from field to field with a new mouse click or the tabulator key.

A new line will be appended when you confirm the sample size with the <ENTER> key.

In this case the **Method** field remains empty as the determinations are to be carried out with the current method.

Save sample data silo: the lines of a sample data silo will be deleted after the corresponding determination has been completed. If you would like to use a sample data silo several times then it is a good idea to save it.

This is done by clicking on [Action] in the main dialog and then selecting **Save sample data silo** in the selection list that appears. Then enter the memory location (only "card 1" or "card 2" possible), the group and the file name and click on [Save].



→ TIP 4

5 Carrying out a titration



Carry out a further three titrations as described in section 3.2. The sample data silo will be processed and a report will be produced after each determination.

→ TIP 6

4 Tips

You have already learned some of the important functions of the Titrando system. This section is intended to present some more interesting options of this titration system. In section 2 and section 3 you will find references for these tips.

Detailed explanations can be found in the Instructions for Use for PC Control / Touch Control.

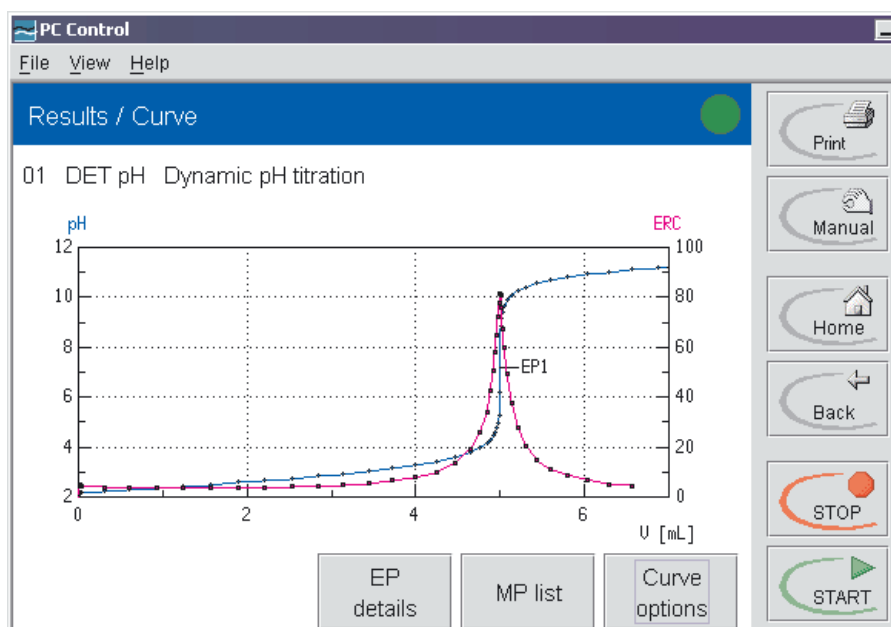
TIP 1 Stirrer rate

The **801 Magnetic Stirrer**, the **803 Ti Stand** and the **802 Rod Stirrer** with **804 Ti Stand** are controlled completely by the PC Control software. The standard stirring rate is set to 8, the middle of the range.

If you want to alter the stirring rate in a method then first optimize it under **Manual / Stir** and enter the value under **Edit parameter** (e. g. DET) / **Edit command / Stirrer**.

TIP 2 Modify curve display

Under **Results / Curve / Curve options** you can modify the curve display, e. g. by selecting a second quantity for the y2 axis (in this case ERC, only for DET) and, in addition, have the measuring points displayed:



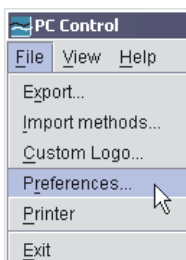
This is also possible in the live display. Just click on [View] during the titration if you want to modify the display of the measured values or the curve directly.

TIP 3 Recalculation

The results of the current determination can be recalculated if the evaluation parameters have been changed.

Recalculation can be triggered by [Recalculate] directly from **Results**.

TIP 4 Define memory location



Apart from the internal memory, data (e. g. methods) can also be stored in extra specified directories on the computer. These are known as "Card 1" and "Card 2" and can be directories on a hard disk, a network drive or any removable storage medium. This permits a similar file management to the use of memory cards with the Touch Control.

In the menu **File / Preferences** you can alter the corresponding paths.

TIP 5 Save determination automatically

You can automatically save determinations by activating this option under **Edit parameter / Method options / Save automatically**.

You can then reload the corresponding results under **Results / More det. data / Load/Save / Load**.

TIP 6 Result silo

The results of up to 200 determinations can be stored in the result silo. Select the required results under **Edit parameter / CALC / Edit command** and activate the option **Save result in result silo** under **Edit / Result options / More options** for each result.

Under **Results / Result silo** now you can see a result for each determination and with **Details** any additional result of the selected determination is also displayed.