



l o n a n a l y s i s

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PC Control

Program version 1.0

**For controlling
808 and 809 Titrandos**

Tutorial

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Although all the information given in the tutorial manual 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 manual for the PC Control software for operating a Titrande 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**

The first things that you will learn are the important steps for the configuration of your titration system.

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

You load a method, start the titration and see the result on the screen.

- **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**

Some of the most important possible ways of using the Titrande system are briefly described. In section 2 and section 3 you will find references (→**TIP**) for these tips.

Detailed information about the way that the Titrande system works and its operation can be found in the online help system and in the corresponding Instructions for Use:

- Installation Instructions for 808 Titrande and 809 Titrande
- Instructions for Use for Touch Control / PC Control
- Instructions for Use for 806 Exchange Unit
- Instructions for Use for 800 Dosino or 807 Dosing Unit
- Tutorial Manual for Touch Control

1.1 Requirements

1.1.1 Equipment

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

- **808 Titrand** with **806 Exchange Unit** or **809 Titrand** with **800 Dosino** and **807 Dosing Unit**
- Computer with **PC Control Software**
- **801 Magnetic Stirrer** or **804 Ti Stand** with **802 Rod stirrer**
- **Titrant** $c(\text{NaOH}) = 0.1 \text{ mol/L}$ (carbonate-free)
- **Sample** 0.1 M HCl
- 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 Instruction for 808 Titrand and 809 Titrand**. The installation of the PC Control software is described in the **Instruction for Use of the PC Control Software**.

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 tubing
5. Connect the Dosino (if present)
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 an 809 Titrand 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 the internal dosing drive of the 808 Titrand.

1.2 Preparations

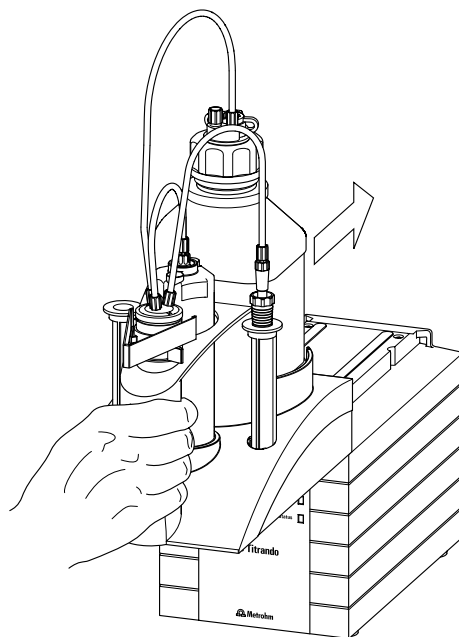
1 Equip the exchange unit or Dosino with titrant

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 (808 Titrande)

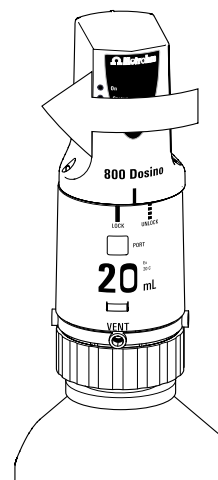
Attach the exchange unit to the 808 Titrande.

Slide it onto the guide rail of the Titrande from the front and push it back until it reaches the stop:



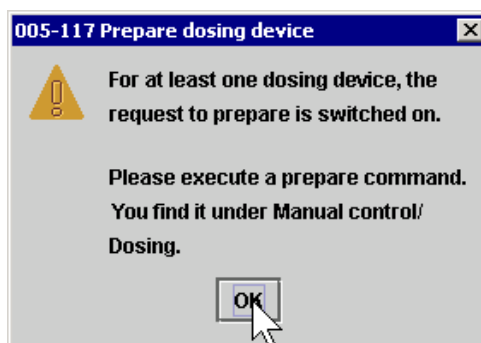
Attach the Dosino to the dosing unit (809 Titrande)

Screw the Dosino onto 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).



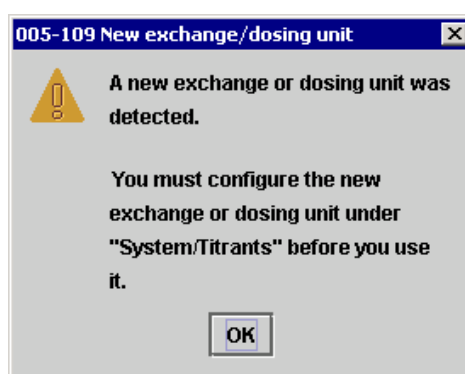
3 Start PC Control

Start the **PC Control** program on your computer. During the system test the following message appears, which should be confirmed with a click on [OK]:



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

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

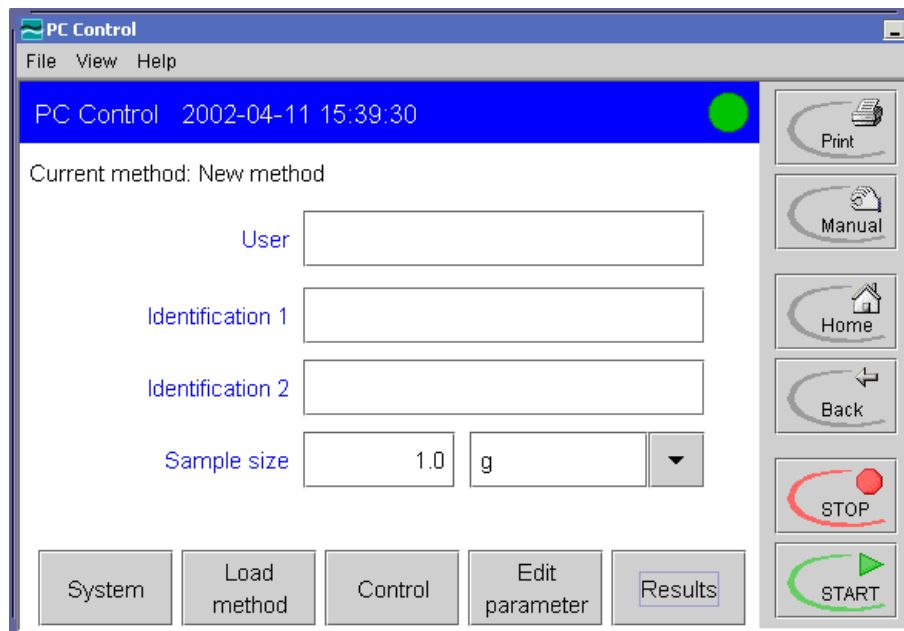


This message must also be confirmed with [OK]. The configuration of the new exchange or dosing unit will be carried out in one of the next steps.

If the datachip of the exchange or dosing unit already contains titrant data then you will be asked whether this data is 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 Touch Control titrant list and can be changed on the datachip.

4 Main dialog

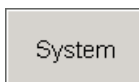
After initialization has been carried out the program desktop opens and shows this program window:



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 [System],...[Results] change their function with the current dialog. They mainly are used to change to a new dialog. Further **Buttons** are used for activating certain functions.



You will use **input fields** for editing numbers and text.

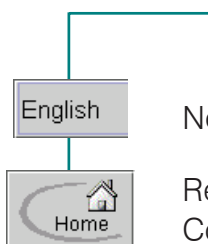
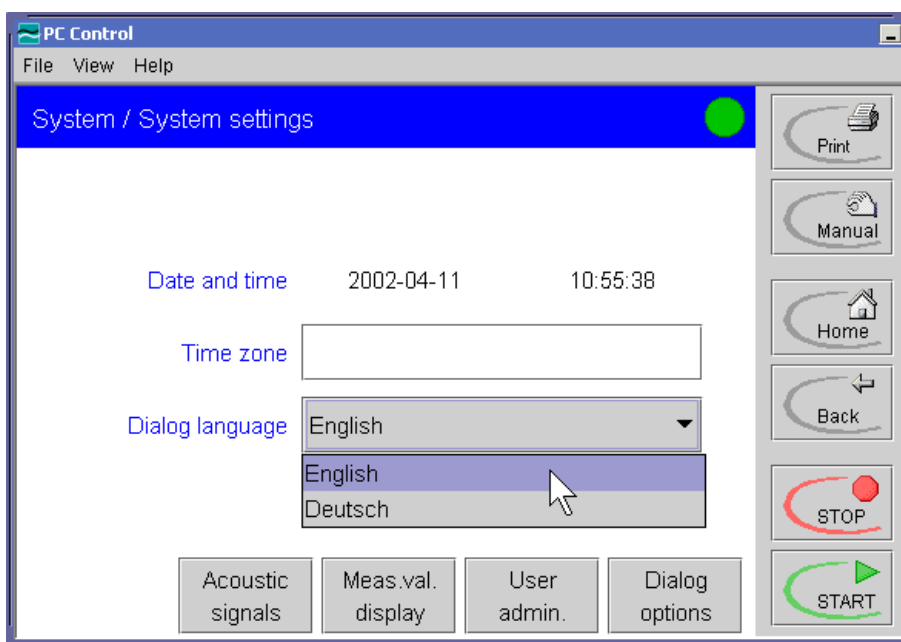
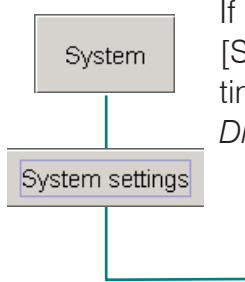
5 Check date and time

In the blue status line at the upper margin of the main dialog the current date and time are shown.

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

6 Set the dialog language to "English"

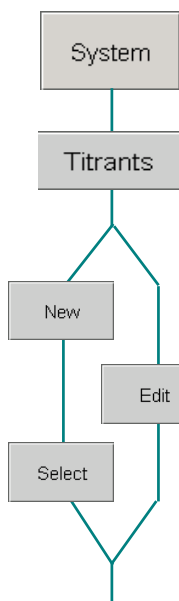
If necessary, you may set the dialog language to "English". Click on the [System] button and in the following selection click on [System settings]. This opens the **System / System settings** dialog. Open the *Dialog language* selection list with a mouse-click.



Now choose the entry **English**.

Return to the main dialog with the fixed key [Home], close the PC Control program and start it up again to make the alteration effective.

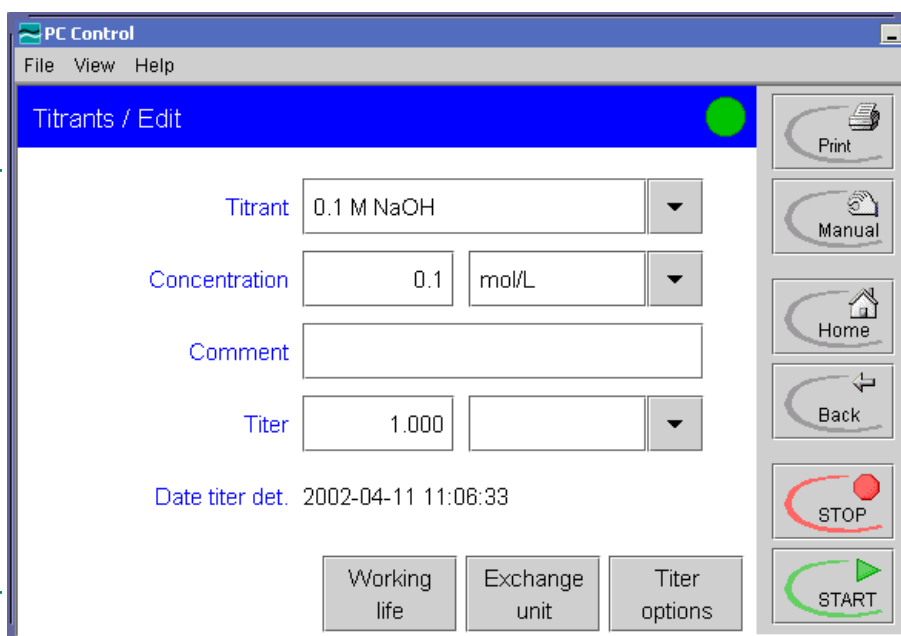
7 Configure a new titrant



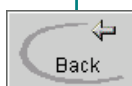
Configure the new titrant under **System / Titrants**.

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 adapted with [Edit]:



Here you can name the **Titrant** as being **0.1 M NaOH**. In the **Concentration** field enter the titrant concentration: **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

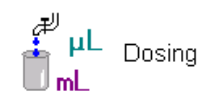


You now have an intelligent exchange unit (IEU) or dosing unit (IDU) available at Dosing device 1 with the titrant 0.1 M NaOH. In this example the cylinder volume is 20 mL, but may be different in your system.

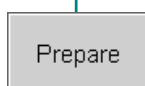
8 Prepare the dosing device



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**. Use the mouse to click on [Dosing].

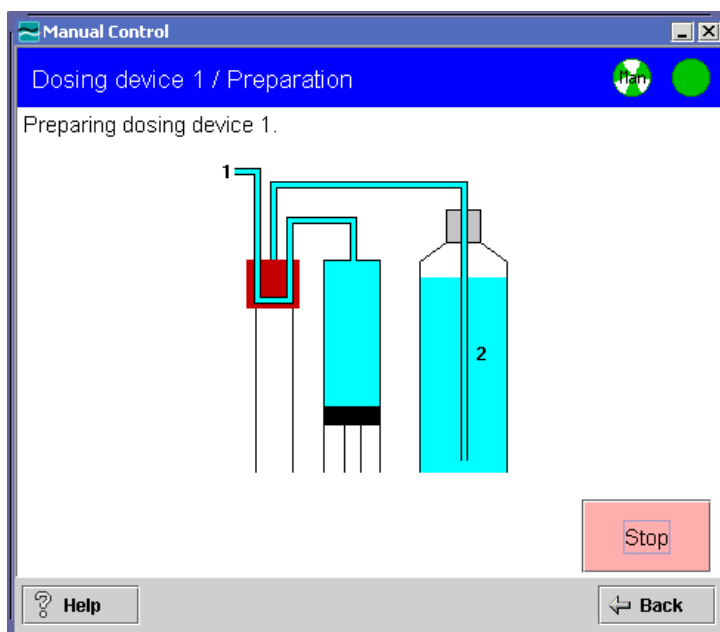



The most important titrant data is shown; click on [Prepare].



The **Splash warning** which now appears informs you that the buret tip of the dosing device is pointed into a container which can accommodate several times the selected cylinder volume.

After this message has been confirmed with [Yes] the dosing cylinder will be emptied and refilled. 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.



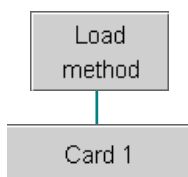
Close the **Manual Control** window with a click on the 'X' in the top right-hand corner.

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

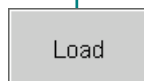
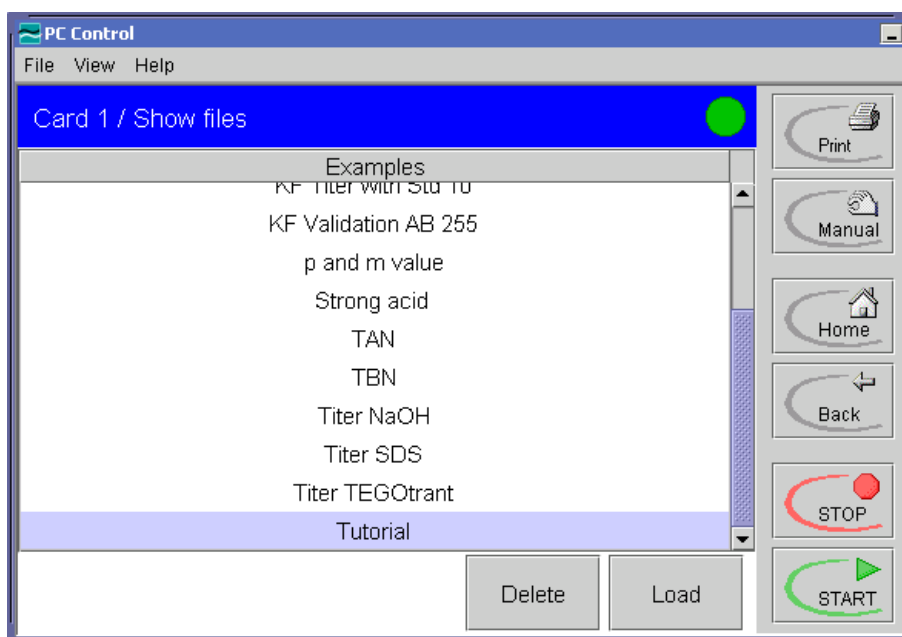
2 Acid/Base titration

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



In the main dialog click on [Load method]. In the group **Examples** select the method **Tutorial**:



Click on [Load].

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

2 Add hydrochloric acid

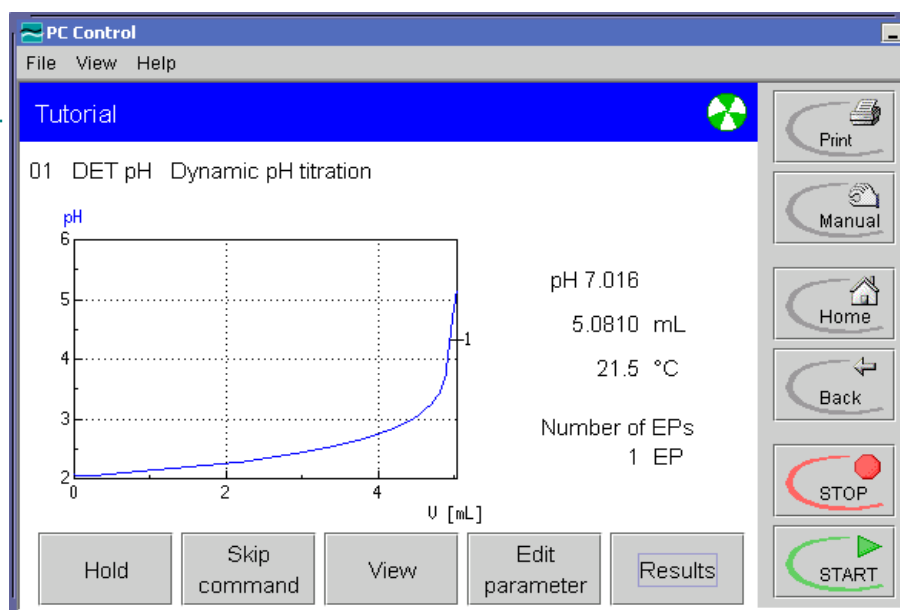
➔ **TIP 1**

In a 100 mL beaker place 50 mL dist. H₂O and 5 mL 0.1 M hydrochloric acid. Then immerse the pH electrode in the solution.

3 Start the titration

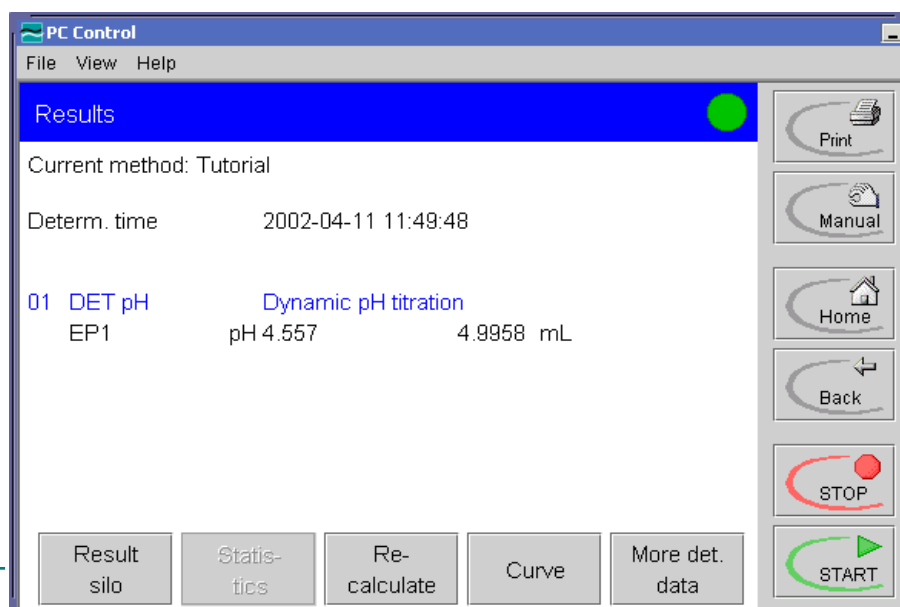


In the main dialog click on [START]. The titration starts with the determination of the initial measured value. After this the running titration is shown in the live display:



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 CO_2 content (CO_3^-) of the H_2O (dist.) or the NaOH used an additional equivalence point EP2 may also be detected.

→ TIP 2

To show 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.

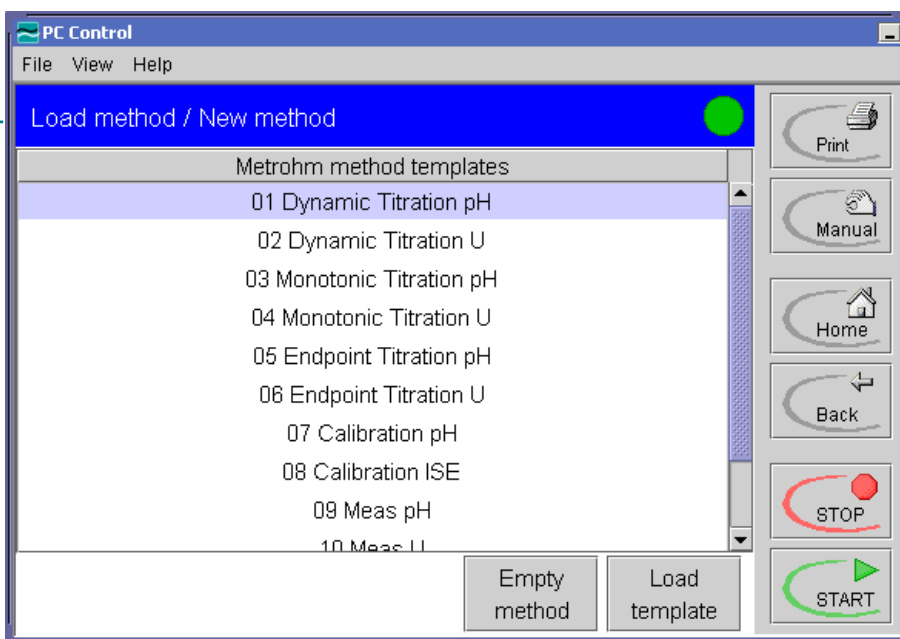
3.1 Creating methods

1 Create a new method

Load method

New method

The easiest way of creating a new method is by the adaptation of 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

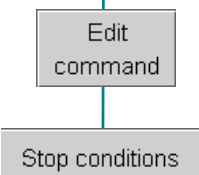
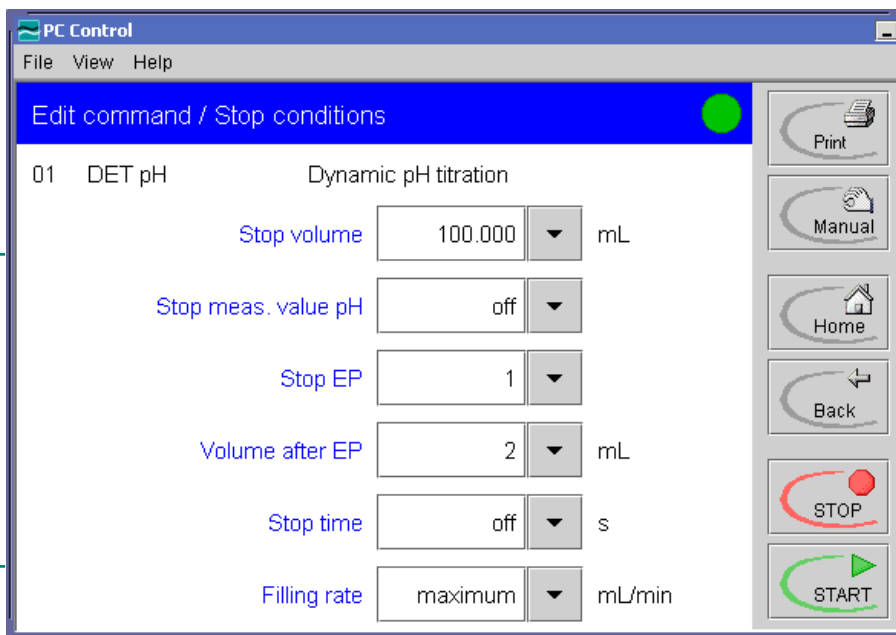
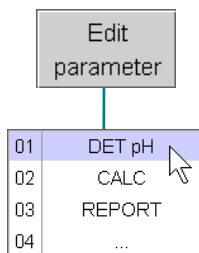
You have loaded the basic skeleton of a method for pH titration with dynamic titrant addition, whose commands can be viewed with [Edit parameters]:

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

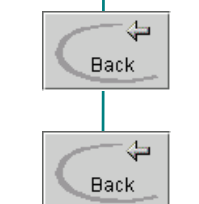
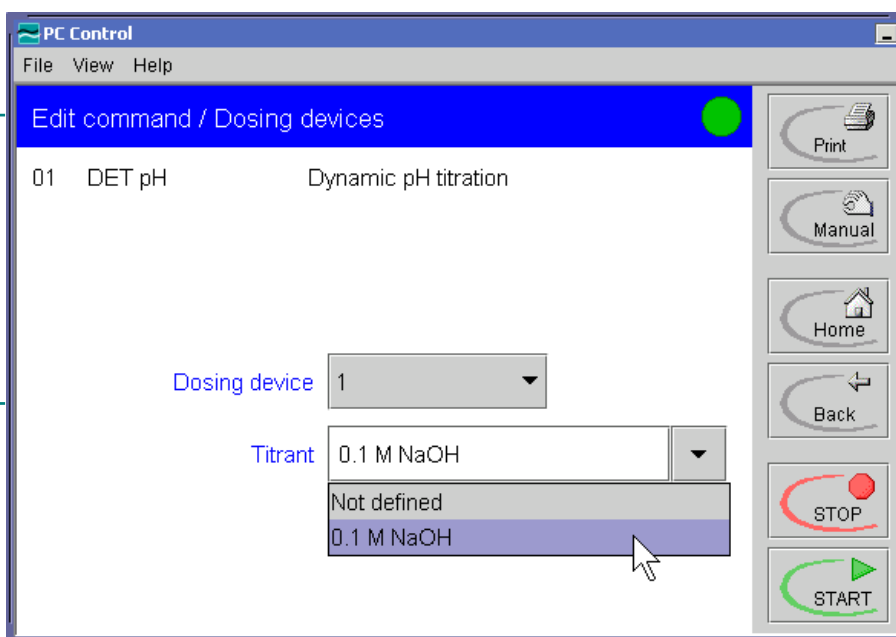
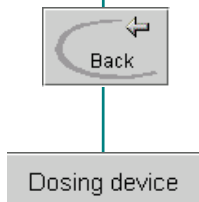
Individual parameters must still be edited.

2 Edit method parameters

01 DET pH / Stop conditions: in this case the titration is also to be ended when 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**). Adapt these parameters accordingly. The stop volume should be retained for safety reasons or adapted to suit the volume of the titration vessel.



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



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.

Edit command

Select **CALC** in line 2 and create a new result calculation with [Edit command] and [New] as follows.

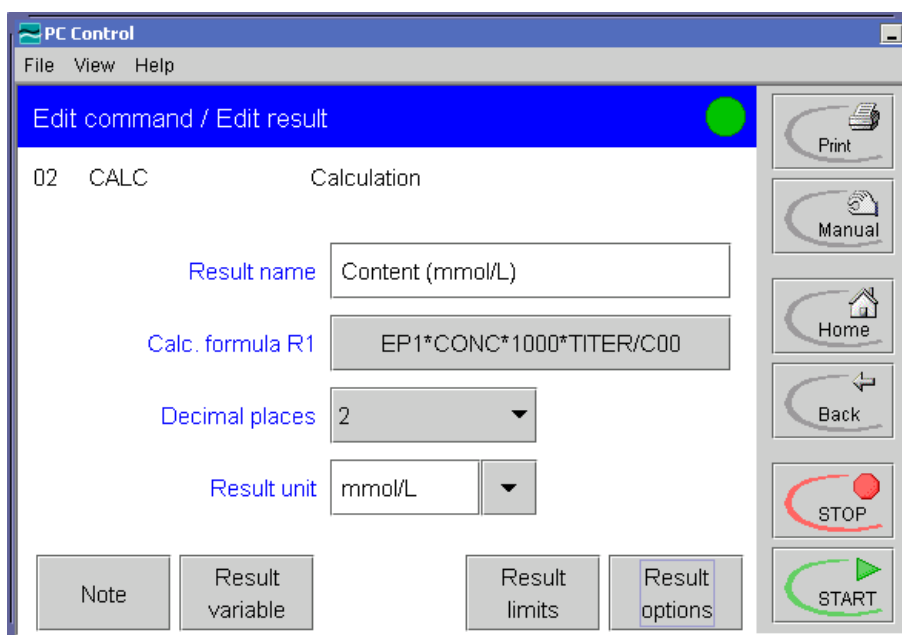
New

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

Metrohm result templates
Content (mmol/L)

Load template

Next



Home

The result R1 is calculated from the following quantities:

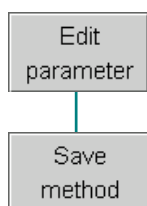
- EP1:** volume of the titrant at equivalence point 1 [mL]
- Conc:** concentration of the titrant [mol/L]
- 1000:** concentration conversion factor, mol/L to mmol/L
- TITER:** titrant titer
- C00:** sample size [mL]

→ TIP 3

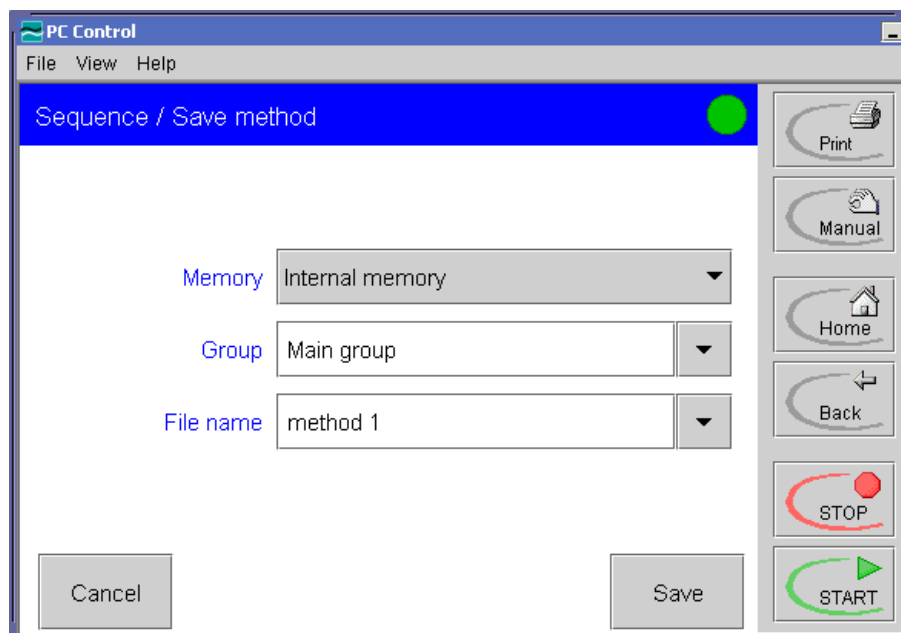
The **sample size** is entered in the corresponding field in the main dialog before the start of the titration. You can also define an automatic request for this value with a REQUEST command or its transfer from a connected balance at the start of a method sequence (see PC Control Instructions for Use).

03 Report: the third command in the method sequence describes the report output on the Windows standard 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 **Parameters / Sequence / 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 respective input field, you edit the group name or file name.

→ TIP 4

You will get a selection list containing further existing groups or file names by clicking on the small triangle on the right side of the input field.

3.2 Titrating

1 Carrying out a titration

→ TIP 1

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

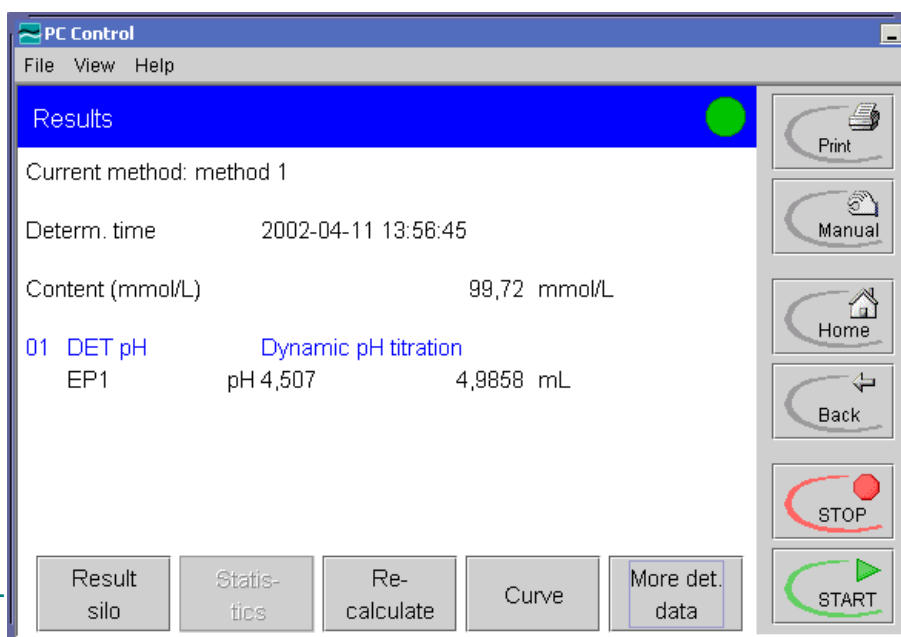
As the method sequence contains an automatic report printout on the connected printer please ensure that the connection is functioning and that the printer has been configured correctly.



First enter the **Sample size** (5 mL) in the main dialog and 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	Serial number Printed	Program version 1.0 2002-04-11 13:58:04
Result report		
Determination	Method method 1 Modified on 2002-04-11 13:55:03 version 2 Method status saved Determin. time 2002-04-11 13:56:45 Status of deter. original Sample number 1 User	
Sample data	Sample size 5 mL	
01 DET pH	Dynamic pH titration	
Titration	EP1 pH 4,507 4,9858 mL Stop EP reached	
Results	Content (mmol/L) 99,72 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 the volume of titrant added, U [mL], ranging from 0 to 6 with major ticks every 2 units. The curve starts at a low pH (around 2) and remains relatively flat until approximately 4.5 mL. At this point, there is a sharp, nearly vertical increase in pH, reaching a plateau of approximately 11. A label '1' is placed at the inflection point of this steep rise, which corresponds to the endpoint (EP1) mentioned in the text above.</p>		

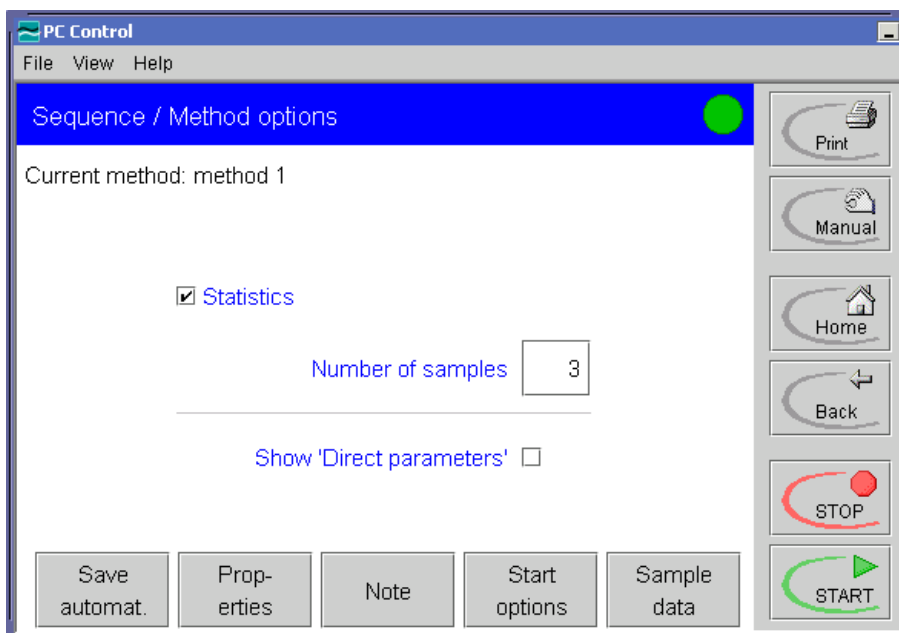
3.3 Statistics and sample data silo

1 Prepare statistics

Edit parameter

Method options

For a statistical evaluation of several results activate statistics under **Parameters / Sequence / Method options**:



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

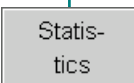
You do not need to return to the main dialog every time with [Back] or [Home] in order to start a measurement. Start the following titration directly from here with [START].

2 Carrying out titrations for statistics

Prepare the electrode and the titration vessel for a new measurement and carry out the titration as described in Section 2 three times. In the main dialog before each titration you must enter a sample identification under **Identification 1** or **2** and the sample size under **Sample size**.



3 x



After each titration a report will be printed out and the result shown. If at this point you return to the main dialog with [Home] then you will see how the determinations are counted for the statistics:

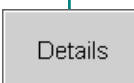
Statistics: 1 of 3

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

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

Current method: method 1
Determinations 3 of 3

Result name	Mean
Content (mmol/L)	99.80 mmol/L



Now click on [Details].

Further statistical data and the individual results will be shown:

PC Control
File View Help

Statistics / Details

Result name: Content (mmol/L) SMN1
Mean 99,80 mmol/L n=03
s +/- 0,112 mmol/L
s rel 0,11 %

No.	Sample size	Result
1	5 mL	99,93 mmol/L
2	5 mL	99,72 mmol/L
3	5 mL	99,76 mmol/L

Buttons: Print, Manual, Home, Back, STOP, START, Sample data, Determ. on/off, Result on/off

3 Print statistics



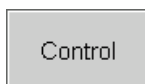
Statistics overview

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

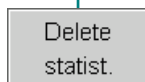
Click on **Statistics overview**, for example.

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

4 Sample data silo



Sample data silo

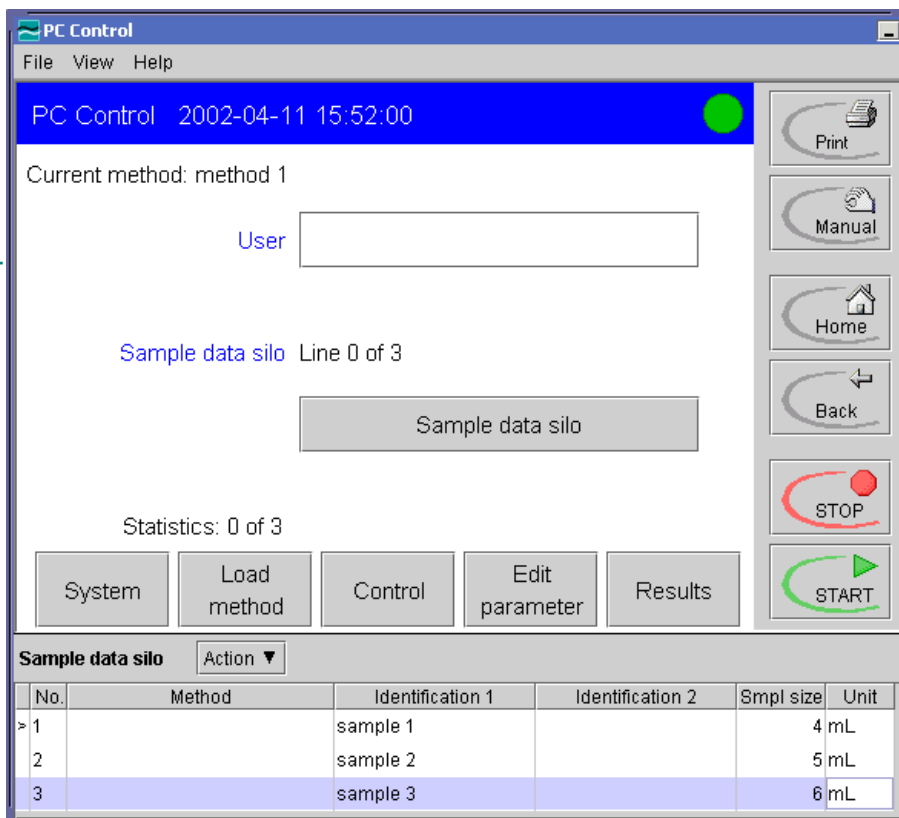


Sample data silo

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

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

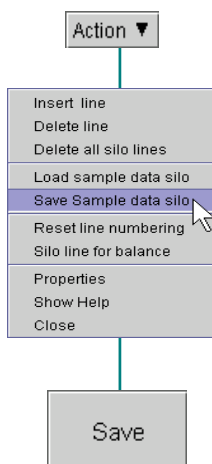
Then click on [Sample data silo] in the main dialog. The empty Sample data silo will now be shown below the program window. Enter some sample data as described below.



Enter sample data: activate the particular input field with a mouse-click and change from field to field with a new mouse-click or the tab 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, 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 other 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 of the PC Control software.

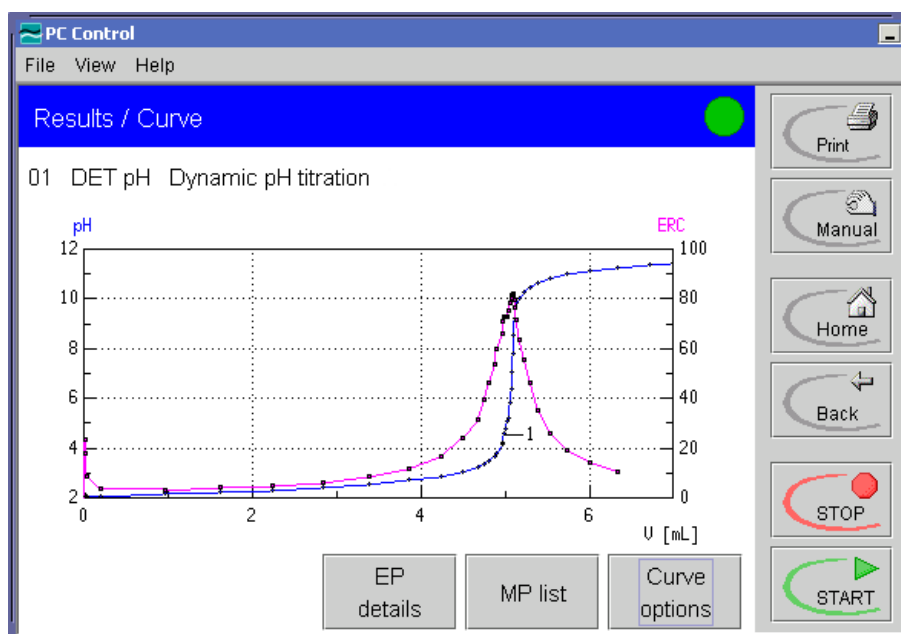
TIP 1 Stirrer rate

The **801 Magnetic Stirrer** and **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 parameters / DET/MET/SET / Edit command / Stirrer**.

TIP 2 Change curve presentation

Under **Results / Curve / Curve options** you can change or extend the curve presentation, e.g. by selecting a second quantity for y2 (in this case ERC, only for DET) and additionally show the measuring points:



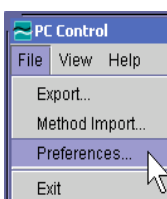
This is also possible in the live display. Just tip on [View] during the titration, if you want to change the presentation of the measured value or curve directly.

TIP 3 Recalculation

The results of the current determination can be recalculated if the evaluation parameters are 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. During the saving of a file and in the File manager these are known as 'Card 1' and 'Card 2'; 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 whole determinations by activating this option under **Parameters / Sequence / Method options / Save automatically**.

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

TIP 6 Result silo

Results of the calculation of up to 99 determinations can be stored in the result silo. This is done by selecting the required results under **Edit parameters / CALC / Edit command** and then activating under **Edit / Result options / More options** the item **Save result in result silo** for each result.

Now you can see under **Results / Result silo** a result for every determination and with **Details** the other results of the selected determination are also shown.