The typographic conventions used in this handbook are given below.

Italic Type

Italic type is used for user defined variables, for example, Enter a *filename* means type the name of your file. *Italic type* is also used for emphasis and titles of handbooks, for example you use *Installing and Using Your UV-Visible Operating Software* handbook to install your software.

Keys

When a key on the keyboard is referred to in this handbook, it is written inside a small box, like the following: ![enter key]

The direction keys are the arrow keys on your computer’s keyboard. These keys, ![Up], ![Down], ![Left], and ![Right], allow you to select different options and to move the cursor on your screen.

Keyboard Entries and Screen Items

When an item that appears on the screen is included in the text or when the instructions call for you to type in a specific letter, word or phrase, the information is presented in this type, for example:

Type INSTUV and press ![Enter].

Most keyboard entries are completed by pressing ![Enter] (the same as Return on other keyboards). A plus sign (+) used between two keynames indicates that those keys must be pressed at the same time. A comma between two keynames indicates that those keys are pressed sequentially.

Softkeys

This software is softkey driven, meaning that you must press a function key or click on a softkey to start an action. The softkeys appear at the bottom of the...
screen. The function keys used by this software are the keys $\text{F1}$ through $\text{F10}$ on your keyboard.

In this handbook, the softkeys are shown in small boxes:

- **Scan 1** and **Measure 1**

The small boxes with round corners, for example, $\text{F10}$, show the function key on the keyboard. The boxes with shading, for example, $\text{Exit 10}$, show the current label for the softkey. All softkey labels include the function key number in the label. For example, if the softkey label is $\text{Scan 1}$, a scan is taken when you press $\text{F1}$ function key on the keyboard.

"Cross References"

It is sometimes necessary to refer to another section of the handbook, for example use "Installing the Software" in Chapter 1 in your *Installing and Using Your UV-Visible Operating Software* handbook for installation instructions. When no chapter number is given then the section is in the same chapter. You can easily find the section using the contents list.

Other Information

**Number Pad.** Use the $(\text{Num Lock})$ key to switch between the arrow keys and numbers when using the number pad.

**System Reset.** It may be necessary to reset the computer system. This is done by simultaneously pressing the keys $(\text{Ctrl}) + (\text{Alt}) + (\text{Del})$ or by turning the computer off and then after a few seconds on again.

**Disk Drive Letters.** In dual flexible disk systems, the upper drive is identified by the letter A and the lower by B. For hard disk systems the disk may or may not be partitioned. The first drive of a hard disk is C.
Notes are indicated like this one. Read this information, it might be helpful or necessary before continuing.
This chapter contains all the commands and their full syntax for the quantification program. The first part of the chapter has a summary of the commands grouped according to type and the second part has the complete details of the commands arranged alphabetically.

## Definitions

<table>
<thead>
<tr>
<th>Command name</th>
<th>Command</th>
<th>Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>A complete instruction to the software. A command typically consists of a command name and one or several parameters; in many cases, the command name only can be a complete command (see also below, &quot;Defaults&quot;).</td>
<td></td>
</tr>
<tr>
<td>Command name</td>
<td>The first part of a command. It may consist of more than one word; words are separated by a blank, e.g. Shell to DOS.</td>
<td></td>
</tr>
<tr>
<td>Parameters</td>
<td>Follow a command name. Parameters specify how exactly a command has to be executed. A parameter can be one of the following:</td>
<td></td>
</tr>
<tr>
<td></td>
<td>- Value or simple keyword like on, off, tabular etc.</td>
<td></td>
</tr>
<tr>
<td></td>
<td>- General string, can contain any character except &quot;.&quot;</td>
<td></td>
</tr>
<tr>
<td></td>
<td>- Command string, contains one or more subcommands and their parameters.</td>
<td></td>
</tr>
</tbody>
</table>
Defaults

In some cases where you do not enter a parameter, the software assumes one automatically; this is the default parameter.

Subcommand

Part of a command string; has a 3 character name and can have parameter(s).

Command string

A special string parameter for a command containing optional subcommands in any order.

Command line

One line, can have one or multiple commands, separated by a semicolon.

Command line display

This is a line on your computer's screen (just above the softkey labels), either displaying the commands in execution (line has a blue background color) or showing the commands as you are typing them using the keyboard (red background color).

Comment

Can be appended to a command line preceded by ".

Command Summary

Command Line

You can enter commands through the keyboard by typing the command, including any parameters if required, and pressing Enter ('keyboard mode'). Alternatively you can use the menu system ('menu mode'), but not all commands/subcommands are supported by the menus supplied with the software (see also "User Interface" in this chapter). Commands can also be entered from a file (see "Run Method" in this chapter). The maximum number of characters in one command line is 32767.
Command Input

The most convenient and the typical way of entering commands is the menu mode. The default setting for the keyboard mode is off.

To turn on the keyboard mode, press a printable key on the keyboard. The prompt Command: is displayed and highlighted, and the background color of the display line turns red. The maximum number of characters in the keyboard mode is 255. You can only turn on the keyboard mode if the highlight is on one of the softkeys, indicating the idle status.

How are Commands Presented in this Handbook?

Read the following information carefully, it describes how commands are presented.

- Command names are printed in uppercase and lowercase for easy reading.
- A command name can be followed by parameters. Parameters are printed in uppercase and lowercase characters for easy reading.
- A command name and its parameters are separated by a slash (/,|\).
- Command names can consist of more than one word. Words are separated by spaces, treated as normal characters.
- Additional spaces can proceed a command name or follow it before the slash.
- If you can specify only one of several options, the options are separated by a vertical bar, |.
- Multiple commands are separated by a semicolon (;).

Parameter

There are three basic types of parameters, simple, general string and command string parameters. Simple parameters must be alphanumeric as described later in this section, and may not include one of the following characters / \ | , ; " and space. General string parameters are always in quotation marks. They can include special characters. Command string parameters
are interpreted by the software and need to follow the syntax described later in this chapter.

Parameters are specified after the slash following the command name. Single or multiple parameters can be specified as well as no parameter at all. Multiple parameters are separated by one of the following characters: space /,\||. Multiple spaces between parameters are treated as a single separator. All of the other parameter separators are treated as one separator each. Commas and spaces are also combined for easy reading. If you can specify only one of several options, the options are separated by a vertical bar, |. When square brackets are nested, parameters in inner brackets can only be specified if the parameters in the outer square brackets are specified.

Parameters must be specified in a fixed order.

Multiple parameters may be optional or required.

Default parameters may be hardcoded or they can be settings, which are loadable with a parameter file.

In case of a setting the optional parameter modifies the current setting.
Entering Commands Correctly

Read the following information carefully, it is important that you know how to enter commands with the correct syntax.

- You can use uppercase or lowercase characters or a mixture of both.
- You must separate the command name from the first parameter by a valid separator, which can be one of the following characters /,|\.
- You may use any number of spaces elsewhere except within the command names, and parameters.
- Do not type the square brackets that are documented in the command syntax to indicate optional parameters.
- All parameters within an instruction, even if they are not specified, must be separated by one of the following characters /,|\.
- You do not need to type the commas at the end of the command if there are only optional parameters following and you do not want to specify them.
- When you give new values to optional parameters, enter them in the specified order.
- When you enter a file name, use the complete path and file name unless the file is in the current data directory. If you do not specify an extension for the file name the software adds the appropriate extension automatically.
- When entering text, use quotation marks, " " , if you want to use the symbols: , ( ) [ ] / + ! ; | or a space.
- Text for component names, and other standard and sample information is case sensitive. Spaces at either end of the names are removed.
- When you have typed-in the command and any parameters, press Enter.
Analytical

Accesses all analytical settings parameters which are relevant for the quantitative calculations.

Syntax

Analytical /1..4,"[AMD SCA|MCA|OFF][;]
[CCT 1..4][;][CMD MLH|LSQ][;]
[DOR 0..20][;][PDG 0..5][;]
[DSM 1..31][;][DAX <deltax>][;]
[A1F <Wfrom>][;][A1T <Wto>][;]
[A2F <Wfrom>][;][A2T <Wto>][;]
[A3F <Wfrom>][;][A3T <Wto>][;]
[A4F <Wfrom>][;][A4T <Wto>][;]
[R1F <Wfrom>][;][R1T <Wto>][;]
[R2F <Wfrom>][;][R2T <Wto>]

Parameter | Description
---|---
1..4 | The analytical method number to be accessed.
"..." | Command string. The analytical settings string. Each parameter in that string changes a single setpoint in the calculations.

Command string

Subcommand | Parameter | Description
---|---|---
AMD | SCA | The subcommand AMD (Analytical Method) specifies whether a single-component analysis (SCA), a multicomponent analysis (MCA) or nothing (OFF) has to be performed. In the last case all other subcommands/parameters are irrelevant.
MCA | OFF |
### Analytical

<table>
<thead>
<tr>
<th>Sub-command</th>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>CCT</td>
<td>1..4</td>
<td>You can specify the calibration curve type with a parameter. The parameter can be 1 to 4, (1 = Beer's law, 2 = linear with offset, 3 = quadratic, 4 = quadratic with offset). The default type is 1, this is also the only valid type in MCA.</td>
</tr>
<tr>
<td>CMD</td>
<td>MLH</td>
<td>The calculation method for maximum likelihood (MCA) or least squares analysis (SCA or MCA).</td>
</tr>
<tr>
<td>DOR</td>
<td>0..20</td>
<td>The derivative order is valid as an integer in a range from 0th to 20th derivative. Its default is 0 for absorbance.</td>
</tr>
<tr>
<td>PDG</td>
<td>0..5</td>
<td>The polynomial degree (PDG) for smoothing and derivatives can be selected in a range from 0 to 5. For derivatives a polynomial degree of at least 1 is required. In general, a polynomial degree of 3 (cubic) is recommended to be able to fit inflection points. The default polynomial degree is 0.</td>
</tr>
<tr>
<td>DSM</td>
<td>1..31</td>
<td>The number of data points used in the smoothing algorithm are specified with DSM (data smoothing). Only odd integers in the range from 1 to 31 points are allowed. The default is 1.</td>
</tr>
</tbody>
</table>
## Analytical

<table>
<thead>
<tr>
<th>Sub-command</th>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>DAX</td>
<td>(&lt;\text{deltax})&gt;</td>
<td>With DAX (delta X) you specify the data density (that is, data interval) in [nm] for the specified ranges. It is a positive single precision floating point number greater than zero. The default is 2 nm.</td>
</tr>
<tr>
<td>A1F</td>
<td>(&lt;\text{Wfrom})&gt;</td>
<td>All the (&lt;\text{Wfrom}&gt;) and (&lt;\text{Wto}&gt;) parameters are wavelength settings in [nm]. A maximum of four analytical ranges is possible. These ranges are specified as single precision numbers. If no range but a single value is to be used, the (&lt;\text{Wto}&gt;) parameter is set to zero. If a possible range is not to be used both parameters are set to zero. If the parameter is not specified the old setting remains active. As a default setting all wavelengths settings are set to zero (this creates an error if no wavelength is actively set and forces the user to select at least one wavelength).</td>
</tr>
<tr>
<td>A1T</td>
<td>(&lt;\text{Wto})&gt;</td>
<td>All of the (&lt;\text{Wfrom}&gt;) and (&lt;\text{Wto}&gt;) parameters are wavelength settings in [nm]. A maximum of two reference ranges is possible.</td>
</tr>
<tr>
<td>R1F</td>
<td>(&lt;\text{Wfrom})&gt;</td>
<td></td>
</tr>
<tr>
<td>R1T</td>
<td>(&lt;\text{Wto})&gt;</td>
<td></td>
</tr>
</tbody>
</table>
Analyze

Calculates quantitative results according to the analytical function settings and the calibration coefficients for all of the samples in the sample buffer.

Syntax

Analyze ["<fname>"|"- Display -", [tabular|all], [<dfactor>], [<limit>], ["<fmask>"]]

Parameter Description

"<fname>" or A valid file name "<fname>". Default extension is .QRS. With "<fname>" the results are stored in the file with that name. If an existing file name "<fname>" is specified, the quantitative results will be appended to that file. With "-Display-" the results are displayed on the screen. Additional "-Display-" parameters can be used to specify how the result will be displayed.

- tabular|all The default result presentation is the tabular form. Options are tabular (short) or all.

- <dfactor> A dilution factor, results are multiplied by this factor. The default is 1.

- <limit> A confirmation tolerance in percent. The confirmation tolerance is switched off by specifying a tolerance of 0%. The default is 1%.

- "<fmask>" A format mask, a fixed format for all results. The default is automatic formatting, i.e. fixed format mask for all results. See Appendix C for details.

No parameter The current output channel is used for storage or display of results.

Requires valid calibration.
## Autosampler

Sets and executes the autosampler parameters.

### Syntax

Autosampler \[/"\[ADV \langle positions\rangle\] \[;\] \[NDL up\|down\] \[;\] \[PRB sample\|wash\]\]"

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>&quot;...&quot;</td>
<td>Command string</td>
</tr>
<tr>
<td>No parameter</td>
<td>The current parameters in the parameter set are used. If parameters are specified they also modify the current parameter set.</td>
</tr>
</tbody>
</table>

### Command string

<table>
<thead>
<tr>
<th>Subcommand</th>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>ADV</td>
<td>\langle positions\rangle</td>
<td>The number of vials to advance. The number must be an integer of the range 0 to 32767.</td>
</tr>
<tr>
<td>NDL</td>
<td>up</td>
<td>The needle position, up or down.</td>
</tr>
<tr>
<td></td>
<td>down</td>
<td></td>
</tr>
<tr>
<td>PRB</td>
<td>sample</td>
<td>Determines whether the probe is in the sample or in the wash position.</td>
</tr>
<tr>
<td></td>
<td>wash</td>
<td></td>
</tr>
</tbody>
</table>
Blank

Takes a reference measurement according to instrumental settings, no output and no display.

Syntax

Blank

Parameter

None

A valid Blank is required for absorbance measurements. If no Blank was measured before a sample or a standard measurement an HP 8452A Error RUNTIME is generated.
Calibrate

Checks valid data set and Analytical Function settings of standards. Calculates calibration coefficients.

**Syntax**

Calibrate

**Parameter**

None

An error will be generated if the calibration process fails.

A valid calibration is the prerequisite for an analysis. The calibrated status is indicated on the Method Summary screen together with the number of components in the standards.
Calibration Curve

Calibration Curve

Draws a calibration curve, if SCA is selected, or all calibration curves using all standards in the standard buffer on the graphics screen.

Syntax

Calibration Curve [/1|2|3|4] [,1|2|3|4] ...

Parameter | Description
---|---
1 ... 4 | Selected calibration curves are displayed.
No parameter | All calibration curves of an SCA method are overlaid. In case of an MCA method an error message is displayed. Also, if the system is not calibrated an error message is displayed.
Change Directory

Changes directory.

Syntax

Change Directory /"<pname>"

Parameter Description

"<pname>" Pathname including drive.

The drive and/or directory is changed according to the
path name specified.
Cursor

Sets the cursor on the current graph (sample or standard spectra) and displays a numerical readout of the current cursor position.

Syntax

Cursor [/<nm>]

Parameter Description

<nm> Specified wavelength position in nm.

No parameter Cursor at the middle of the wavelength axis.

If no spectral graph display is active the command is terminated without error.
Delay

System waits until the specified time has elapsed.

Syntax

Delay /<seconds>

Parameter | Description
---|---
<seconds> | Time in seconds.

Note

A delay cannot be aborted. For synchronization with external events better use the trigger command.
Delete Files

Deletes all files specified in the list.

Syntax

Delete Files /*<fname1>", "<fname2>" */ ...

Parameter Description

"<fname1>", List of file names.
"<fname2>"

Note

In Run Method mode files are deleted without warning!

Wildcards are allowed to delete multiple files. Before the files are deleted, a box with the question "Delete File(s) ?" and the possibility to cancel the delete operation is displayed.
# Delete Samples

Delete Samples

## Syntax

Delete Samples \[/[<sid1>][,<sid2>] ... \]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;sid1&gt;, &lt;sid2&gt;</td>
<td>Sample identification. From 1 to the maximum number of samples in memory. Enter L for last sample only.</td>
</tr>
<tr>
<td>No parameter</td>
<td>All samples in memory.</td>
</tr>
</tbody>
</table>

The samples are removed from the sample buffer. The buffer size is reduced, the data is reorganized if required.
Delete Standards

Deletes standards.

Syntax

Delete Standards [/[<sid1>] [, <sid2>] ... ]

Parameter | Description
--- | ---
<br>\(<sid1>\), \(<sid2>\) | Standard identification. From 1 to the maximum number of standards in memory. Enter L for last standard only.

No parameter | All standards in memory.

The standards are removed from the standard buffer. The buffer size is reduced, the data is reorganized if required. The calibration status is no longer indicated on the Method Summary screen.
Display

Allows you to switch all screen output on or off.

Syntax

Display /on|off

Parameter  Description

on|off  On restores the screen and rechecks the mouse. Off turns the display off.

Switching the display off may be useful in an automated environment. In that state all commands can be executed and the input is monitored.

In the automated (Run Method) mode no error messages are displayed if the display is switched off.

Note

In case of a fatal error the menu system is displayed automatically. However, if the system is running in an endless loop (e.g. if the instrument is not powered on) nothing is displayed. If this happens the menu system can be displayed by pressing (ESC), (ENTER), typing Display /on and pressing (ENTER).
Error Log

Appends all error messages to the specified file along with time and date, if a valid file name (“<fname>”) is specified.

Syntax

Error Log /on,"<fname>" | off

Parameter Description

on, "<fname>" Turns error logging on. "<fname>" can be a new file name or an existing name of an error log file. Default extension is .QLG.

off Turns error logging off.

Error logging is especially useful in an unattended Run Method mode, when the display is switched off. Logging errors and printing them after the automation mode is finished is the only way of getting the information about errors occurred during the automated mode.

Note

In the case of multiple commands in a command line the execution of all commands following the one where the error occurred are ignored.
<table>
<thead>
<tr>
<th>Exit</th>
<th>Terminates program execution. Files are closed, data in memory are lost.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Syntax</td>
<td><strong>Exit</strong></td>
</tr>
<tr>
<td>Parameter</td>
<td>None</td>
</tr>
<tr>
<td>Note</td>
<td>All data (standard, sample, current parameter set) which are not stored will be lost.</td>
</tr>
</tbody>
</table>
## Graphics Copy

Prints or plots to a file or a device.

### Syntax

```
Graphics Copy /PR|PL [, [<dtype>], ["<channel>"], [<lmargin>], [<linpage>]]
```

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>PR</td>
<td>PL</td>
</tr>
<tr>
<td><code>&lt;dtype&gt;</code></td>
<td>The device type (<code>&lt;dtype&gt;</code>) specifies the printer (0 = HPPCL, 1 = Epson, 2 = PaintJet) or plotter type (not used, only HPGL plotter supported).</td>
</tr>
<tr>
<td><code>&quot;&lt;channel&gt;&quot;</code></td>
<td>A valid DOS file or device.</td>
</tr>
<tr>
<td><code>&lt;lmargin&gt;</code></td>
<td>The left indent margin must be greater than or equal to zero and defaults to 6.</td>
</tr>
<tr>
<td><code>&lt;linpage&gt;</code></td>
<td>The lines per page parameter <code>&lt;linpage&gt;</code> must be greater than 20 and defaults to 62. A maximum number of 32767 can be used to suppress the insertion of page headers when storing to a file.</td>
</tr>
</tbody>
</table>

If no device type and/or channel is specified the defaults stored in the configuration file are used.

The `<lmargin>` and `<linpage>` parameter are only valid as printer parameter.
Handling

Inserts single or multiple tasks automatically before (Input) or after (Return) a measurement.

**Syntax**

Handling /Blank|Standard|Sample, Input|Return

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Blank</td>
<td>Standard</td>
</tr>
</tbody>
</table>

The type of measurement.

Sample Handling must be ON to execute the Handling commands with the Measure command.

The execution point in time.

Single or multiple commands can be defined for execution before (Input) or after (Return) a measurement.

The current Handling information is displayed for editing in the command line display. A maximum of 255 characters can be entered. The only restriction is that a comment must not be used in the Input part.

A Run Method command is executed after all Handling commands are executed.

In the case of multiple commands in a command line the execution of all commands following the one where an error occurred are ignored. An error in Handling commands may aboard before the Measure command is executed.

The Handling command is not logged to a method file.
HP-IB

Syntax

HP-IB [/DMA|HP8452,<address>|HP89090,<address>]

Parameter

DMA

Description

The DMA keyword allows to switch on the DMA mode (DMA channel 3) if the amount of data to be transferred is greater than 300 bytes. Because some operating systems themselves are using DMA channels or manipulate the memory, DMA transfer can fail!

HP8452,<address>
HP89090,<address>

The first digit of the <address> represents the interface board address (0 ... 7, the HP-IB interface) and the last two digits represent the HP-IB device address (0 ... 32). A valid address is stored as the current address and all further communication with the specified device (HP8452A or HP89090A) is directed to the current address. When exiting and reentering the quantification program, the current address is loaded from the configuration file. This allows to use multiple instruments with the software. In that case the appropriate instrumental parameters should be sent to each of the instruments before the first measurement is made. Also a separate blank has to be triggered for each of the HP 8452As installed.

No parameter

The current settings are used and the HP-IB interface board is reinitialized in non-DMA mode.
HP-IB

This is i.e. required when a hangup with an HP-IB plotter occurs.
**Instrumental**

Specifies all of the instrumental parameters in a way similar to the primary instructions sent to the instrument.

**Syntax**

```
Instrumental [/"[LMP 0|1][;][SHU 0|1][;]
   [TRG <Mode>,<Meas flag>,<Delay>][;]
   [MSK <Bits>][;][VRN 0|1][;]
   [FMT <Mode>,<Format>][;]
   [INT <Mode>,<Gain>][;]
   [TIM <Integ>,<Interval>,<Readings>,<Delay>][;]
   [WAV <Mode>,<Lambda1>[,<Lambda2>][,..<Lambda20>]][;]
   [REF <Integ>,<Output>]]"
```

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>&quot;...&quot;</td>
<td>Command string</td>
</tr>
</tbody>
</table>

**Command string**

<table>
<thead>
<tr>
<th>Sub-command</th>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>LMP</td>
<td>0</td>
<td>Lamp state, specifies whether the lamp is to be turned on (1) or off (0).</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>SHU</td>
<td>0</td>
<td>Shutter mode, specifies whether the shutter is to be closed between repeat measurements (0) or opened (1).</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>TRG</td>
<td>&lt;Mode&gt;</td>
<td>Trigger</td>
</tr>
</tbody>
</table>

0..2 specifies the trigger detection mode. 0 disables trigger detection, 1 enables trigger detection on a 0 to 1 transition of the trigger line, and 2 enables trigger detection on a 1 to 0 transition of the trigger line.
<table>
<thead>
<tr>
<th>Sub-command</th>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>&lt;Meas flag&gt;</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>&lt;Delay&gt;</td>
<td>0.0..99999.9 specifies the delay time, in seconds, between the time the trigger signal is detected and the start of the measurement cycle (if meas flag is 0, then this is not applicable), the corresponding trigger status bit is also set at this time.</td>
</tr>
<tr>
<td>MSK</td>
<td>&lt;Bits&gt;</td>
<td>Service request Mask, 0 ... 63, specifies the decimal value of bit pattern that is to serve as a mask for the status bits &lt;Bits&gt;.</td>
</tr>
<tr>
<td>VRN</td>
<td>0</td>
<td>Variance mode, specifies whether variance data is to be calculated (1) or not (0).</td>
</tr>
<tr>
<td>VRN</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>FMT</td>
<td>&lt;Mode&gt;</td>
<td>Format record length 0</td>
</tr>
<tr>
<td></td>
<td>&lt;Format&gt;</td>
<td>0</td>
</tr>
<tr>
<td>Sub-command</td>
<td>Parameter</td>
<td>Description</td>
</tr>
<tr>
<td>-------------</td>
<td>-----------</td>
<td>-------------</td>
</tr>
<tr>
<td>INT</td>
<td>&lt;Mode&gt;</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Intensity</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0..4 specifies the type of data that will be collected during the next measurement cycle.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Mode Data Type</td>
</tr>
<tr>
<td></td>
<td></td>
<td>0 Absorbance</td>
</tr>
<tr>
<td></td>
<td></td>
<td>1 Intensity at current gain</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2 Intensity at fixed gain</td>
</tr>
<tr>
<td></td>
<td></td>
<td>3 Dark current at current gain</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4 Dark current at fixed gain</td>
</tr>
<tr>
<td>TIM</td>
<td>&lt;Gain&gt;</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0 to 15 specifies the fixed gain to use for modes 2 or 4, this parameter is ignored otherwise.</td>
</tr>
<tr>
<td>TIM</td>
<td>&lt;Integ&gt;</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Timing</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Integration time (0.1 to 25.5), specifies the period of time, in seconds, that the beam through the sample is integrated on the diodes.</td>
</tr>
<tr>
<td>TIM</td>
<td>&lt;Interval&gt;</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>0.1 to 99999.9 specifies the time, in seconds, between successive measurements.</td>
</tr>
<tr>
<td>TIM</td>
<td>&lt;Readings&gt;</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>1 to 999999 specifies the number of measurements that are to be taken during the next measurement cycle.</td>
</tr>
<tr>
<td>Sub-command</td>
<td>Parameter</td>
<td>Description</td>
</tr>
<tr>
<td>-------------</td>
<td>-----------</td>
<td>-------------</td>
</tr>
<tr>
<td>WAV</td>
<td>&lt;Delay&gt;</td>
<td>0 to 99999.9 specifies the delay time, in seconds, between receiving the instruction to measure and the start of the measurement cycle.</td>
</tr>
<tr>
<td>WAV</td>
<td>&lt;Mode&gt;</td>
<td>0 or 1 specifies the measurement mode. 0 specifies that a wavelength range is to be measured, 1 specifies that a list of selected wavelengths is to be measured.</td>
</tr>
<tr>
<td>WAV</td>
<td>&lt;Lambda xx&gt;</td>
<td>190 to 820 for the standard instrument, 190 to 510 for option #002, 470 to 1100 for option #003) specifies the wavelengths to be measured. If mode was 0, then lambda1 specifies the starting wavelength and &lt;lambda2&gt; specifies the ending wavelength of a range. If mode was 1 then up to 20 lambdas may be specified as selective wavelengths to measure.</td>
</tr>
<tr>
<td>REF</td>
<td>&lt;Integ&gt;</td>
<td>Reference measurement Integration time (0.1 to 25.5).</td>
</tr>
<tr>
<td>REF</td>
<td>&lt;Output&gt;</td>
<td>0 or 1 specifies whether output measure data is to be generated. Optional; if omitted, the value is retained from the last REF instruction.</td>
</tr>
</tbody>
</table>
Instrumental

Any order can be used to set one, multiple or all of these parameters. Not all possible combinations of parameters can be used. The full meaning of these allowed parameters are described in detail in the *Interfacing and Programming Guide* (part number 08452-90006). If no parameter is specified the actual settings are downloaded to the instrument.

Note

There is no check of the validity of parameters when a command is entered. If the instrument is communicating, it generates errors for invalid parameters; if not, only an HP-IB timeout is generated. In order to avoid errors, it is strongly recommended for the less experienced operator to change instrument parameters only through the menu mode.
Message

Displays a message box on the screen.

Syntax

`Message ["<text>", [<style>], [<CInd>], [<row1>], [<col1>], [<row2>], [<col2>]]`

Parameter | Description
---|---
"<text>" | A text string with multiple lines can be generated. Use the "|" as new line character. The default is no text (""").

/style> | The style parameter is 1 for left adjusted and 4 for centered text. Styles 11 and 14 for printing in reverse mode. 11 is left adjusted, 14 is centered. The default is 4.

<CInd> | The color index can be selected from 0 to 3; default is 3. The color index refers to one of the four color settings in the configuration file "CONFIG52.DAT".

<row1> <col1> | The box size can be specified in character positions by the upper right corner (<row1>, <col1>) and the lower left corner (<row2>, <col2>). The range of rows is 25 to 1 and the range of columns is 1 to 79. The defaults are <row1> = 7, <col1> = 10, <row2> = 14, <col2> = 70. If the text does not fit into the specified box, it is truncated.

You must press <OK> to terminate the message command.

Note

If the display is switched off (spacebar) or (Enter) can be used to continue.
Method Summary

Switches from graph display back to method summary display.

Syntax

Method Summary

Parameter

None

If the system is in the calibration curve graphics and the status changes to not-calibrated, the Method Summary screen is shown automatically. Also, with the display on, the Method Summary screen is shown when the command Shell to DOS is entered.
Multicell Transport

Sets and/or reads the multicell transport parameters.

Syntax

Multicell Transport ["CEL <cpos>,<steps>"]

Parameter | Description
---|---
"..." | Command string
No parameter | The current parameters in the parameter set are used.

Command string

Subcommand | Parameter | Description
---|---|---
CEL | <cpos> | cell positions 1 to 7 or H (Home).
 | <steps> | step positions 0, 51 ... 6650.

If parameters are specified they also modify the current parameter set.

The "CEL" subcommand controls the multicell transport movement. If only the cell position <cpos> is specified the transport is moved to this position. If both the cell position and the steps (<steps>, 51 ... 6650) are specified a new absolute position in steps is defined and the transport moves to this position. If a step position 0 is specified, the predefined positions (HP 8452A internal) are used.

Note

After using step positions (51 ... 6650) for precision movement of the transport, you must reset <steps> to 0.
Multicell Transport

Note

To ensure the correct transport position at the beginning of an automated run, you must specify also the first position of the multicell transport; otherwise the run starts with the current position. A good practise is to start with the Home position before specifying other cell positions.
Print Calibration

Prints a calibration report to a file or a device.

Syntax

Print Calibration [/[,<dtype>], ["<channel>"],
[<lmargin>], [<linpage>]]

Parameter Description

<dtype> The device type (<dtype>) specifies the printer (0 = HPPCL, 1 = Epson, 2 = PaintJet).

"<channel>" A valid DOS file or device for the report.

<lmargin> The left indent margin must be greater than or equal to zero and defaults to 6.

<linpage> The lines per page parameter <linpage> must be greater than 20 and defaults to 62. A maximum number of 32767 can be used to suppress the insertion of page headers when storing to a file.

If no device type and/or channel is specified the defaults stored in the configuration file are used.

A calibration report includes standard spectra, the analytical parameters and the standard table. In SCA method calibration coefficients and function results are added to the report.

To obtain a calibration report, the system must be in the calibrated status.

If a calibration file name is displayed in the Method Summary screen, it will be reported together with the time and date.
Print Parameter

Prints all actual parameters to the specified channel.

Syntax

Print Parameter [/["<channel>"], [<margin>], [<linpage>]]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>&quot;&lt;channel&gt;&quot;</td>
<td>A valid DOS file or device for the report.</td>
</tr>
<tr>
<td>&lt;margin&gt;</td>
<td>The left indent margin must be greater than or equal to zero and defaults to 6.</td>
</tr>
<tr>
<td>&lt;linpage&gt;</td>
<td>The lines per page parameter &lt;linpage&gt; must be greater than 20 and defaults to 62. A maximum number of 32767 can be used to suppress the insertion of page headers when storing to a file.</td>
</tr>
</tbody>
</table>

The default is the printer configured for the system. By specifying this parameter you can direct the output elsewhere. In addition you can specify optional parameters for the left indent and the lines per page.

The length of a parameter report is dependant on the actual settings, e.g. only wavelengths settings other than zero are reported, sample handling commands may or may not be programmed, etc.
Recall Calibration

Recall Calibration loads a calibration including a complete parameter set. The standards and parameter currently in memory are lost and overwritten by the standard data and the parameter set stored in the calibration file.

Syntax

Recall Calibration /"<fname>"

Parameter | Description
----------|------------------
"<fname>"  | A valid file name. Default extension is .QCL.

Recall calibration deletes the old standards first, then loads the new standards, loads the new parameters and calculates the Analytical Functions for the standards, then for the samples. When no error occurred, the status in the Method Summary screen is set to Calibrated. If the samples currently in memory cannot be analyzed with the new analytical parameters, the status will be Uncalibrated. In order to avoid this, it is preferable to store all sample spectra on a file, then delete all samples in memory before recalling a calibration. When reloading the samples now, an error will be generated if a spectrum is incompatible, so you can identify this spectrum (see also "Recall Samples"). Another advantage is that an out-of-memory error, by loading too many samples, can be avoided.

If a wildcard (*,?) is used in the file name it acts as a filter for a selection box of file names. The selection box is displayed and the system waits for a selection of a file name by the operator. This makes the recall calibration task interactive and can be used in a 'semi' automated method, to prompt the user to enter a file name before the automated analyses are performed. For example, you can program an automated method for an autosampler where at the beginning the operator is asked to select the parameter file for this specific set of samples.
Recall Parameter

Recall Parameter

- Loads a parameter set.

**Syntax**

Recall Parameter

/"<fname>" [,all|analytical|configuration]

**Parameter**

- `<fname>`
  - A valid file name. Default extension is .QSP.

- all|analytical|configuration
  - Allows extraction of either the analytical part or the configurational part of the parameter set. The default is the complete set, that is, all.

If a wildcard (*) is used in a file name it acts as a filter for a selection box of file names. This makes the recall parameter task interactive and allows you to load different parameter sets in an automated run (see also "Recall Calibration").

The parameter recall can be skipped by pressing **[ESC]**. In this case the current parameter set remains unchanged.
Recall Samples

Recalls a spectrum or spectra to be analyzed.

Syntax

Recall Samples /"<fname1>" [,","<fname2>" ] ...

Parameter Description

"<fname1>" , List of valid file names. Default
"<fname2>" extension is .WAV.

Recall Sample does the following:

- Increments Sample counter.
- Allocates Sample data header memory according to the
  header information.
- Gets header.
- Allocates memory for Sample raw data.
- Gets raw data.
- Allocates memory for analytical data if a calculation
  method is activated.
- Calculates Analytical Function values.

If a wildcard (*.?,) is used in a file name it acts as a filter
for a selection box of file names. This makes the recall
of the samples task interactive and allows you to load
different data in an automated run (see also "Recall
Calibration").

Note

Even if the calculation for a spectrum fails, other
spectra will be recalled and the calculations continue.
When all spectra are analyzed, a single error message is
generated. Remove the sample which generates the error
(use Analyze to - Display - to get the indices of the
sample(s)) and reanalyze the data set.
Recall Samples

Note

If you import a wavelength (.WAV) file originally stored with the HP 89532A general scanning or the HP 89531A UV-Vis operating software and store the spectrum again with the quantification software, the file type (FTYPE, see Appendix B) is changed from 11 to 1 and the pump/sipper settings are lost.
Recall Standards

Recalls a spectrum or spectra for calibration.

**Syntax**

```
Recall Standards /"<fname1>" [,"<fname2>" ] ... 
```

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>&quot;&lt;fname1&gt;&quot;</td>
<td>Valid file names. Default extension is WAV.</td>
</tr>
<tr>
<td>&quot;&lt;fname2&gt;&quot;</td>
<td>WAV</td>
</tr>
</tbody>
</table>

Recall Standards does the following:

- Increments Standard counter.
- Allocates Standard data header memory.
- Gets header.
- Allocates Standard raw data memory according to the header information.
- Gets raw data.
- Allocates memory for analytical data if a calculation method is activated.
- Calculates Analytical Function values.

If a wildcard (*) is used in a file name it acts as a filter for a selection box of file names. This makes the recall of the standards task interactive and allows you to load different data in an automated run (see also "Recall Calibration").

**Note**

If the calculation fails (e.g. a recalled spectrum does not have the right wavelength range), other standards are continued to be recalled and a single error message is generated after all standards have been loaded. You have to remove the 'bad' spectrum before you can get a valid calibration. The best way to find the 'bad' standard(s) is to display the standard spectra (Graphics, Standard Spectra) and to use the cursor to find its index. You can then delete the standard (Edit, Delete Standard) and recalibrate.
Record Method

Writes all steps performed in an analysis to a file on disk in append mode, for automation purposes.

Syntax

Record Method /on,"<fname>"|off

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>on,</td>
<td>Turns method recording on or off.</td>
</tr>
<tr>
<td>&quot;&lt;fname&gt;&quot;</td>
<td>Default extension is .QAU.</td>
</tr>
<tr>
<td>off</td>
<td></td>
</tr>
</tbody>
</table>

With Record Method on, all commands are stored in the specified file.

If Sample Handling is switched on, all Handling commands are recorded in the menu driven system and complete methods are copied onto the file when a method is executed while the recording is on.

After Record Method is switched off, the generated method can be executed using the Run Method command with the file name "<fname>".

Note

In the case of multiple commands in a command line the execution of all commands following the one where an error occurred are ignored.
Report

Generates a report out of the stored analytical results.

**Syntax**

`Report /"<fname>", [tabular|all], [<dfactor>], [<limit>], ["<fmask>"], ["<channel>"], [<lmargin>], [<linpage>]`

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><code>&lt;fname&gt;</code></td>
<td>A valid results file name. Default extension is .QRS.</td>
</tr>
<tr>
<td>tabular</td>
<td>all</td>
</tr>
<tr>
<td><code>&lt;dfactor&gt;</code></td>
<td>The dilution factor, used to multiply all the results with. The default is 1.</td>
</tr>
<tr>
<td><code>&lt;limit&gt;</code></td>
<td>The confirmation tolerance in percent. The default tolerance is 1%. A confirmation tolerance of zero switches confirmation analysis off.</td>
</tr>
<tr>
<td><code>&lt;fmask&gt;</code></td>
<td>A format mask can be specified for a fixed format report. If no <code>&lt;fmask&gt;</code> is specified a format mask is automatically generated for each sample. If a format mask is specified, a fixed format is used for all results. Especially in a tabular form, results are much easier to compare, if only the significant digits are printed. For specifying a format mask see &quot;Format Mask Selections&quot; in Appendix C.</td>
</tr>
<tr>
<td><code>&lt;channel&gt;</code></td>
<td>The output channel or device. See Appendix D, for more information.</td>
</tr>
<tr>
<td><code>&lt;lmargin&gt;</code></td>
<td>A left margin in a range of 0 to 20 characters.</td>
</tr>
<tr>
<td><code>&lt;linpage&gt;</code></td>
<td>The lines per page.</td>
</tr>
</tbody>
</table>

Result reports are generated from result files. Results can always be added to an existing result file by use of the Analyze command together with the file's name. Appending results in a file allows you to e.g. collect...
results, which you want to compare, over an extended period of time and report all of them in the same table. On the other hand, if a comparison does not make sense because the samples are different, they should be stored in different files.
Rescale

Redraws the content of the current graph (sample spectra, standard spectra or calibration curve) using the new window.

Syntax

Rescale [/<xlow>, <xhigh>, <ylow>, <yhigh>]

Parameter | Description
--- | ---
<xlow>, <xhigh>, <ylow>, <yhigh> | Specified scaling parameters are used and the fix scale status is set.
No parameter | Autoscaling is used and the autoscale flag is set.

Internally for each graph an independent set of scaling parameters is held. The set of parameters used is determined by the current graph (standard spectra, sample spectra, calibration curves).
Run Method

**Run Method**
Runs a method.

**Syntax**
Run Method /"<fname>"

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>&quot;&lt;fname&gt;&quot;</td>
<td>A valid file name. Default extension is .QAU.</td>
</tr>
</tbody>
</table>

If you enter a valid file name, command-input is out of the file instead of user inputs. If a wildcard is used, a filtered selection of automation files in a list box is displayed.

The automation flag is set. This flag is automatically reset on I/O error or EOF in the automation file. In Trace Mode automation can be executed stepwise and aborted if required. Task logging is also applicable in automation mode. This allows you to copy part of automation sequences.

**Note**
If an error occurs during an automated run, the display is automatically switched on if it was switched off.

**Note**
In the case of multiple commands in a command line the execution of all commands following the one where an error occurred are ignored.
Sample

Takes a measurement according to the actual settings of the instrument, data are added to the sample buffer.

Syntax

Sample /["<sname>"], [<conc>], [<stddev>],
["<units>"], ["<solvent>"]]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>&quot;&lt;sname&gt;&quot;</td>
<td>The sample name.</td>
</tr>
<tr>
<td>&lt;conc&gt;</td>
<td>The sample concentration.</td>
</tr>
<tr>
<td>&lt;stddev&gt;</td>
<td>The standard deviation for the concentration of the sample.</td>
</tr>
<tr>
<td>&quot;&lt;units&gt;&quot;</td>
<td>The concentration units.</td>
</tr>
<tr>
<td>&quot;&lt;solvent&gt;&quot;</td>
<td>The solvent name.</td>
</tr>
</tbody>
</table>

To identify a sample in the report, at least a sample name should be entered.
Sample Handling

<table>
<thead>
<tr>
<th>Syntax</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample Handling /on</td>
<td>on/off Sample Handling switched on or off.</td>
</tr>
<tr>
<td>Parameter</td>
<td>Description</td>
</tr>
<tr>
<td>on</td>
<td>off  Sample Handling switched on or off.</td>
</tr>
</tbody>
</table>
Sample Information

Allows you to edit most of the sample header information.

Syntax

Sample Information /<sid>, ["<name>"], [<conc>], [<stddev>], ["<units>", ["<solvent>"]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;sid&gt;</td>
<td>The sample identification.</td>
</tr>
<tr>
<td>&quot;&lt;name&gt;&quot;</td>
<td>The sample name.</td>
</tr>
<tr>
<td>&lt;conc&gt;</td>
<td>The sample concentration.</td>
</tr>
<tr>
<td>&lt;stddev&gt;</td>
<td>The standard deviation for concentration of the sample.</td>
</tr>
<tr>
<td>&quot;&lt;units&gt;&quot;</td>
<td>The concentration units.</td>
</tr>
<tr>
<td>&quot;&lt;solvent&gt;&quot;</td>
<td>The solvent name.</td>
</tr>
</tbody>
</table>

If nothing is specified for a specific parameter no changes are made to these items.

The first parameter is the sample identification <sid> to select a sample. If a string parameter (included in double quotes) is to be cleared a string including a single blank character (" ") can be used. Defaults are always the existing sample headers.
**Sample Spectra**

Displays the raw data for the sample(s) on the graphics screen.

**Syntax**

```
Sample Spectra[/<sid1>, [<sid2>] ...]
```

**Parameter**  

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;sid1&gt;,</td>
<td>The sample identifications. Samples specified in the list are overlaid. The L sample identification can be used for the last sample in the buffer.</td>
</tr>
<tr>
<td>&lt;sid2&gt;</td>
<td></td>
</tr>
</tbody>
</table>

**No parameter**  

All samples are overlaid.
Shell to DOS

Calls the operating system and executes the specified command line.

Syntax

Shell to DOS[/"<comline>"], [continue]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>&quot;&lt;comline&gt;&quot;</td>
<td>The DOS command to execute.</td>
</tr>
<tr>
<td>continue</td>
<td>Sets a continue flag for suppression of the user prompt to quit for continuation.</td>
</tr>
<tr>
<td>No parameter</td>
<td>The DOS command processor is executed. The DOS “Exit” command resumes program execution.</td>
</tr>
</tbody>
</table>

The available memory for a program to be executed from the Shell is shown in the Message line. If this memory is unsufficient, an out of memory error is generated.
Sipper

Executes a sipper function and sets and/or changes the sipper parameters.

**Syntax**

Sipper [/"[DIR cw|ccw][;][TIM <ptime>][;][DEL <dtime>][;][PNO <npump>]"]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>&quot;...&quot;</td>
<td>Command string</td>
</tr>
<tr>
<td>No parameter</td>
<td>The current parameters in the parameter set are used.</td>
</tr>
</tbody>
</table>

**Command string**

<table>
<thead>
<tr>
<th>Subcommand</th>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>DIR</td>
<td>cw, ccw</td>
<td>The pump direction for sample input (cw = clockwise) or sample return (ccw = counter clockwise).</td>
</tr>
<tr>
<td></td>
<td>&lt;ptime&gt;</td>
<td>The pumping time in seconds.</td>
</tr>
<tr>
<td></td>
<td>&lt;dtime&gt;</td>
<td>The delay time after pumping in seconds.</td>
</tr>
<tr>
<td></td>
<td>&lt;npump&gt;</td>
<td>The pump number. Valid pump numbers are 0 .. 4. If a pump number &lt;npump&gt; greater than 0 is specified, the corresponding multiplexed pump control channel of the HP 89078A valve/pump controller is used.</td>
</tr>
</tbody>
</table>

If parameters are specified they also modify the current parameter set.
Note
Specify a pump number other than zero only, if the HP 89078A valve/pump controller unit is used to control one or more pumps.
Standard

Takes a measurement according to the actual settings of the instrument, data are added to the standard buffer.

Syntax

Standard /"<sname>" , <conc> [, [<stddev>], ["<units>"], ["<solvent>"]]

Parameter | Description
---|---
"<sname>" | The standard name. To use a standard for calibration a valid component name as a standard name must be specified along with the standard concentration. If a SCA method is activated, identical component names must be used for all standards. The Sample Information command can be used for that task.

<conc> | The standard concentration.

<stddev> | The standard deviation for the concentration of the standard.

"<units>" | The concentration units.

"<solvent>" | The solvent name.

Note

The standard deviation information of the standard concentration is only used for maximum likelihood calculations. This information cannot be stored in the data file.
## Standard Information

Allows you to edit most of the standard header information.

### Syntax

```
Standard Information /<sid>, ["<sname>"], [<conc>], [<stddev>], ["<units>"], ["<solvent>"]
```

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;sid&gt;</td>
<td>The sample identification.</td>
</tr>
<tr>
<td>&quot;&lt;sname&gt;&quot;</td>
<td>The standard name.</td>
</tr>
<tr>
<td>&lt;conc&gt;</td>
<td>The standard concentration.</td>
</tr>
<tr>
<td>&lt;stddev&gt;</td>
<td>The standard deviation for the concentration of the standard.</td>
</tr>
<tr>
<td>&quot;&lt;units&gt;&quot;</td>
<td>The concentration units.</td>
</tr>
<tr>
<td>&quot;&lt;solvent&gt;&quot;</td>
<td>The solvent name.</td>
</tr>
</tbody>
</table>

If nothing is specified for a specific parameter no changes are made to these items.

The first parameter is the standard identification `<sid>` to select a standard. If a string parameter (included in double quotes) is to be cleared a string including a single blank (" ") can be used. Defaults are always the existing standard headers.

With maximum likelihood calculations, when standards are recalled and the standard deviations of the concentrations should be used for the calculations, the standard deviations have to be entered.
Standard Spectra

Displays the raw data for the standard(s) on the graphics screen.

Syntax

Standard Spectra \[/[(<sid1>), (<sid2>) ... ]\]

Parameter | Description
---|---
<br/>&lt;sid1&gt;, &lt;sid2&gt; | The sample identifications. Standards specified in the list are overlaid. The L standard identification can be used for the last standard in the buffer.
No parameter | All standard spectra are overlaid.
Store Calibration

The software must be in the calibrated state. All standard data in memory along with the current parameter set are stored to disk.

Syntax

```
Store Calibration /"<fname>"
```

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>&quot;&lt;fname&gt;&quot;</td>
<td>A valid file name. Default extension is .QCL.</td>
</tr>
</tbody>
</table>
Store Parameter

Stores all current parameters in ASCII format to disk.

Syntax

Store Parameter /"<fname>"

Parameter | Description
---|---
"<fname>" | A valid file name. Default extension is .QSP.
Store Samples

Stores sample raw data to a file.

Syntax

Store Samples
/<sid1>,"<fname1>"[,<sid2>,"<fname2>"] ...

Parameter Description

<sid1> The sample index in memory.

"<fname1>" A valid file name. Default extension is .WAV.

Store Samples does the following:

- Opens a file.
- Stores sample header and raw data.

Multiple samples can be specified in a list by their indices and a destination file name. The sample to be stored to disk is specified by its index in the sample buffer. Valid indices are 1 ... maximum number of samples, and the L index for the last sample in the buffer.

If entered through the menu, a warning is displayed if a file already exists. In the automated mode (Run Method) files will be overwritten without warning.

To avoid overwriting a file or if you want to use similar file names for a group of spectra you can use an asterisk (*) in the file name. This automatically appends an index to the file name and checks for already existing files. You may only use a single asterisk in the file name to generate indices. File names are limited to 8 characters. For example, using a five character prefix, that is XXXXX*, allows you to store a maximum of 999 different sample spectra files. If an index overflow occurs (in the example of a five characters prefix with the 1000th spectrum), the leading 1 is truncated, generating the zero index (here XXXX000). As with normal file names, an overwrite warning is displayed in the menu or keyboard mode if an index overflow occurs. In the automated mode (Run Method), all further spectra are stored in the file with
zero index. Therefore only the last measured sample spectrum is available in that file.
Store Standards

Stores standard raw data to a file.

Syntax

Store Standards
/<sid1>,"<fname1>"[,<sid2>,"fname2"] ...

Parameter       Description

<sid1>          The sample identification.

"<fname1>"      A valid file name. Default extension is .WAV.

Store Standards does the following:

- Opens file.
- Stores standard header and raw data.

Multiple standards can be specified in a list by their indices and a destination file name. The standard to be stored to disk is specified by its index in the standard buffer. Valid indices are 1...maximum number of standards, and the L index for the last standard in the buffer.

If entered through the menu, a warning is displayed if a file already exists. In the automated mode (Run Method) files will be overwritten without warning.

To avoid overwriting a file or if you want to use similar file names for a group of spectra you can use an asterisk (*) in the file name. This automatically appends an index to the file name and checks for already existing files. You may only use a single asterisk in the file name to generate indices. File names are limited to 8 characters. For example, using a five character prefix, that is XXXXX*, allows you to store a maximum of 999 different sample spectra files. If an index overflow occurs (in the example of a five characters prefix with the 1000th spectrum), the leading 1 is truncated, generating the zero index (here XXXXX000). As with normal file names, an overwrite warning is displayed in the menu or keyboard mode if an index overflow occurs. In the automated mode (Run Method), all further spectra are stored in the file with
zero index. Therefore only the last measured sample spectrum is available in that file.
Temperature Controller

Sets and/or reads the temperature controller parameters.

Syntax

Temperature Controller [/"[SET <settemp>] [:;]
[SEU C|K|F] [:;][PEL on|off] [:;]
[SPE <speed>] [:;][STR on|off] [:;]
[REM on|off]"

Parameter | Description
--- | ---
" ... " | Command string
No parameter | The current parameters in the parameter set are used and downloaded to the instrument after pressing <OK>.

Command string

<table>
<thead>
<tr>
<th>Sub-command</th>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>SET</td>
<td>&lt;settemp&gt;</td>
<td>The cell holder temperature is set with this parameter. Set temperature units.</td>
</tr>
<tr>
<td>SEU</td>
<td>C</td>
<td>Switches the Peltier device on or off.</td>
</tr>
<tr>
<td></td>
<td>K</td>
<td></td>
</tr>
<tr>
<td></td>
<td>F</td>
<td></td>
</tr>
<tr>
<td>PEL</td>
<td>on</td>
<td>The speed for the stirrer. Stirrer switched on and off.</td>
</tr>
<tr>
<td></td>
<td>off</td>
<td></td>
</tr>
<tr>
<td>SPE</td>
<td>&lt;speed&gt;</td>
<td></td>
</tr>
<tr>
<td>STR</td>
<td>on</td>
<td></td>
</tr>
<tr>
<td></td>
<td>off</td>
<td></td>
</tr>
<tr>
<td>REM</td>
<td>on</td>
<td></td>
</tr>
<tr>
<td></td>
<td>off</td>
<td></td>
</tr>
</tbody>
</table>

If parameters are specified they also modify the current parameter set.

The parameters can be specified in any order.

The validity of the parameters is checked by the temperature controller itself. If it is not on-line, no check occurs and a communication error is reported.
Trace Mode

Sets or resets a trace mode flag to allow a stepwise execution and analysis of all parameters used in a command.

**Syntax**

Trace Mode /on|off

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>on</td>
<td>off</td>
</tr>
</tbody>
</table>

This command is not written to a method file in the Record Method mode.

This command works in the menu, the command line and the automated (Run Method) mode. It is particularly useful for checking a running method or recording a method.

It offers additional capabilities:

- In the Record Method mode unwanted actions can be deleted from logging by using the <Skip> function. The command is then executed, but not logged to the file.

- In the automated mode, all parameters can be checked stepwise and the run can be aborted before the displayed command is executed.

**Note**

With a text editor, a Trace Mode command can be written into the method file in order to switch the trace mode on and off automatically during execution (in the Record Method mode, a Trace Mode command cannot be automatically written to a method file).
**Trigger**

Scans the GP-IO input as long as the specified bit pattern, given as a character string, is read.

**Syntax**

```plaintext
Trigger /<pattern> [,<timeout>], [abort|continue]
```

**Parameter**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>&lt;pattern&gt;</td>
<td>One character is used per bit. A '1' of the HP 8452A GP-IO port means no contact closure, a '0' means contact closure, any other character means 'don't care'. The left most character represents the most significant bit (bit 7), the right most character represents the least significant bit (bit 0). The GP-IO port has 8 bits. If less than 8 characters are specified, the leading ones are set to 'don't care'.</td>
</tr>
<tr>
<td>&lt;timeout&gt;</td>
<td>Timeout is specified in seconds, the default is zero. If a timeout greater than 0 is specified, scanning of the GP-IO input is aborted when the pattern was not read and the time has elapsed.</td>
</tr>
<tr>
<td>abort</td>
<td>continue</td>
</tr>
</tbody>
</table>
Trigger together with a timeout of 0, the system halts until the specified pattern is read (i.e. 0 means indefinitely here).
User Interface

Allows you to load different user interfaces.

Syntax

User Interface "<fname>"

Parameter | Description
---|---
"<fname>" | A valid file name. Default extension is .QUI.

If a wildcard (*,?) is used in a file name it acts as a filter for a selection box of file names. This makes the user interface command interactive and allows you to load different user interfaces in an automated run (see also "Recall Calibration").

A new set of menus, items and parameter windows are loaded. The basic structure of this file is label oriented. It is a text file with the menu and parameter window description.

A menu definition line has the following structure:

<menu index>, <item index>, <status>, "<item/menu name>", <shortcut key>.

The menu description is one menu or item per line. The menu description is preceded by the string label "[Menu]". The menu index is related to the softkeys. Therefore its range is 1 to 10. The maximum number of items and/or menus is limited to 15. The item index range is 0 to 15, where 0 is the menu index, not an item. Valid item names are all commands described in this chapter. The status must be one or two. One is without and two is with an added check mark to the item. Only the commands Record Method, Logging, Trace Mode, Error Log, Sample Handling and Display handle check marks. The shortcut key definition is not used.
Example

```
"[Menu]"
1, 0, 1, "Measure", 1
  1 : menu index, menu definition for softkey #1
  0 : menu index, the <menu name> is the softkey label
     1 : status, this line has no check mark
    "Measure" : text, the softkey label
1, 1, 1, "Blank", 1
  1 : menu index, menu definition for softkey #1
  1 : item index, 1st line in the menu
  1 : status, this line has no check mark
    "Blank" : text, the first menu item text
1, 2, 1, "Standard", 1
  1 : menu index, menu definition for softkey #1
  2 : item index, 2nd line in the menu
  1 : status, this line has no check mark
    "Standard" : text, the second menu item text
1, 3, 1, "Sample", 1
  1 : menu index, menu definition for softkey #1
  3 : item index, 3rd line in the menu
  1 : status, this line has no check mark
    "Sample" : text, the third menu item text
```

The example defines the softkey #1, with the label Measure. If the softkey is pressed, the following is displayed:
User Interface

A parameter window definition begins with a string label which refers to a predefined set of parameter entry screens.

The following parameter windows are available:

```
"[Ed8452]" instrument parameter
"[EdAnal]" analytical parameter
"[Ed89090]" temperature controller parameter
"[EdSip]" sipper parameter
"[EdAS]" autosampler parameter
"[EdMCel]" multicell transport parameter
"[EdVal]" valve parameter
"[EdInfo]" sample information parameter
"[PaDel]" delay task parameter
"[PaTrg]" trigger task parameter
"[PaRep]" report task parameter
"[PaPar]" recall parameter options
"[PaRes0]" rescale standards parameter
"[PaRes1]" rescale samples parameter
"[PaRes2]" rescale calibration curves parameter
"[PaHa]" sample handling parameter
"[End]" file termination label
```

A line in a parameter window definition corresponds to a single parameter manipulation field. It can be positioned by the specification of a window row and column anywhere in that window. The parameter window size is determined automatically out of the coordinates and the total field length. When stepping through a parameter window the order in which the definition is given is used. So the first line in the definition corresponds to the first parameter, the second line to the second parameter ... etc. The screen position is not used in stepping from one to another parameter but the sequence in the definition.

The parameter definition line consists of up to 11 parameters and has the following structure:

- Edit field type
  - 0 = on screen entry formatted
  - 1 = select box (directly used as parameter)
### User Interface

2 = toggle box (translated into 0/1)

3 = on screen entry unformatted (scrolling) line

4 = select box (on screen translated into index)

Types 10, 11, 12, 13, 14 generate a string parameter enclosed in quotes.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Window row</td>
<td>1..19.</td>
</tr>
<tr>
<td>Window column</td>
<td>1..76.</td>
</tr>
<tr>
<td>Edit field prompt</td>
<td>String, 60 character maximum.</td>
</tr>
<tr>
<td>Subcommand</td>
<td>3 character fixed length string. If not a subcommand, a zero string (&quot;&quot;) must be specified.</td>
</tr>
<tr>
<td>Parameter index</td>
<td>For a subcommand parameter the position in the list of parameter(s) has to be specified (first index = 1).</td>
</tr>
<tr>
<td>Format mask</td>
<td>To display and cut parameters a format mask according to the basic syntax with up to 60 characters can be specified. The mask determines the result (numerical and string).</td>
</tr>
<tr>
<td>Units</td>
<td>A 15 character maximum string for specifying the units. This can be a zero string for suppression.</td>
</tr>
<tr>
<td>Maximum length</td>
<td>Maximum input length. This is only valid for edit field types 3 and 13 (scrolling fields).</td>
</tr>
<tr>
<td>Default</td>
<td>60 character maximum default, only valid in non subcommand parameters.</td>
</tr>
<tr>
<td>List of valid entries</td>
<td>Only valid in edit field types 1 and 11. 60 characters maximum, otherwise specify zero string.</td>
</tr>
</tbody>
</table>
User Interface

All parameters are specified on one line separated by commas. String parameters are enclosed in quotes.

"[EdInfo]"
string label: the following lines define a sample information parameter window

10, 1, 2, "Sample Name", ",", 1, " \\
10: entry field type; string parameter on screen entry formatted
1: 1st row of window
2: 2nd column of the window, window entry is indented by one character
"Sample Name": edit field prompt
"": this is not a subcommand
1: parameter index; entry ignored because this is no subcommand
"\": format mask; fixed length, 15 character string, indented
": units; no units specified
15: maximum edit field length, entry ignored because edit field type is not 3 or 13
": default entry, none defined
": list of valid entries, entry ignored because edit field type is not 1 or 11

"[End]"
Valves

Switches a valve and modifies the current valve parameters.

Syntax

Valves ["[VNO <number>];[CHA <channel>]"]

Parameter | Description
--- | ---
"..." | Command string.
No parameter | The current parameters in the parameter set are used.

Command string

<table>
<thead>
<tr>
<th>Subcommand</th>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>VNO</td>
<td>&lt;number&gt;</td>
<td>Selects number of the valve, 1 ... 4.</td>
</tr>
<tr>
<td>CHA</td>
<td>&lt;channel&gt;</td>
<td>Selects one of the channels 1 ... 8.</td>
</tr>
</tbody>
</table>

If parameters are specified they also modify the current parameter set.

This command allows to control up to four valves connected to the HP 89078A valve/pump controller. In addition to the valves HP 89052B peristaltic pumps can be controlled via the sipper command. Use the same <number> for the valve and the associated pump.

Note

Do not use the Valves command if no HP 89078A controller unit is connected. The autosampler, if connected, may be damaged!