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SOFTWARE AND CONSULTING FOR INSTRUMENTAL ANALYSIS

VISION*lite* ColorCalc

Software for the Determination of Sample Color Parameters

Operator's Guide

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1 Introduction

VISION*lite* ColorCalc is a PC application software under Microsoft Windows® to scan the spectra of glass, filters and liquid samples with full instrument control and to execute various calculation procedures to numerically describe sample colors. The software provides easy operation at a high degree of flexibility. Thus you can generate sophisticated sample parameters simply and quickly in a routine environment. See: *Evaluation Parameters* 7-1.

Supported Instruments and Hardware

The software communicates with Thermo Scientific® UV/Vis and Vis spectrophotometers of the GENESYS® 10S series with BioMate 3S and Evolution 160S, Evolution® 200 series and Evolution 300. Please see the notes regarding the specific models in *Spectrometer and Accessories* 10-1.

The software runs under current Microsoft Windows® versions. The necessary system components are given in the installation section. See: *Hardware and Operating System Requirements* 2-1.

Provided Calculations

The range of available calculation options includes various parameters for color descriptions and decisions. The parameters generally are defined by international and national standards such as DIN, EN, CIE, JIST, ANSI, etc. See: *Evaluation Parameters* 7-1.

You can also define additional parameters. Naming, output format and other details can be configured.
See the details on the adaptation and generation of parameters in *Adapting the evaluation parameters* 8-1 and *Calculations Window* 5-21.

Spectrum readings can be taken in transmission or in reflectance with dark and white standard correction. See: *Reflectance Measurements* 8-9.

If you should have a need for further calculation parameters or if you would like to propose an improvement for one of the definitions please contact the supplier.

Compatibility to other Software Packages

The software is compatible with the Thermo Scientific **VISION*lite*®** software and with the ***ascanis*** **Reporter-SPX** software.

Previously recorded spectra in various data file formats can be evaluated:

- **VISION*lite*®** spectra can be evaluated offline.
- The software also loads spectra in the JCAMP format.
- Data tables can be imported as well, e.g. generated by Microsoft Office Excel® or by the Thermo Scientific **VISIONpro/security** and **INSIGHT®** software **csv**-files.

For more information see: *Data Formats and Import/Export* 9-1

Reporter-SPX Software

You can additionally install the **Reporter-SPX** application software, which allows customizing reports in a user-defined format. For example, it is possible to place a company logo at the top

of each report page, to add descriptive or sample-specific text information, to integrate additional calculation procedures – like peak detection – as scripts, or to export the report in various formats. See: *Report Configuration* 8-35.

1.1 Text Conventions

The following text conventions are used in this document:

Important
An important note indicates that there are critical problems that could cause any damage or falsification of critical data files.

Note: *A note makes you aware of hints critical for safety and correctness of your data.*

Tip: *This kind of hint is meant for making things easier for you.*

Additionally, the following text conventions are used:

- Keys on the keyboard of your computer are set in square brackets.
  Example: [ENTER], [F1]
- The plus sign between keys indicates that two keys must be pressed in combination.
  Example: [SHIFT] + [A] generates the capital letter A.
- Texts displayed on the screen are given in **bold** characters.
- Variable names of files and directories are given between carrots.
  Example: <Filename>**.txt** indicates files with a special type of filename and the filename extension **.txt**.
- The asterisk * in filenames is a wildcard for any number of alphanumeric characters.
  Example: ***.txt** is any file with the filename extension **.txt**.

Spectrophotometer vs. Spectrometer
The terms ***spectrophotometer*** and ***spectrometer*** are generally considered synonymous. The software's user interface and the software documentation texts generally use the designation *spectrophotometer*. A technical difference is not implied.

2 Installation

2.1 Hardware and Operating System Requirements

The software requires the following hardware system:

- Standard Windows PC or notebook (laptop) with a CD/DVD drive.
- The screen must have a resolution of minimum 1024 x 768 pixels.
- An appropriate interface (RS-232 C (serial), USB or USB with USB-serial converter) must be installed to connect the spectrophotometer to the computer.
- Approximately 20 MB hard disk space are required for operating the software. Moreover, there should be sufficient free additional hard disk space to save data and method files.
- The PC must run a Microsoft Windows® operating system Windows XP, Vista or 7/8/8.1.

2.2 Connecting the Spectrophotometer to the PC

The spectrophotometer models are connected to the PC via RS-232 C interface or USB port. With RS-232C, the COM 1 interface is used as the default interface; alternatively the software can be configured to run with other COM interfaces. This can be selected during installation or during software operation. With a USB port, the appropriate COM port is assigned automatically.

It is recommended to use an interface cable as supplied with the instrument or as recommended by the spectrophotometer supplier. If the PC does not have the required serial interface, alternatively also a USB-to-serial adapter can be checked.

Compatible Instruments and Accessories

The various instruments that can be used with our software application exhibit different technical functions. For example, these include the available wavelength range, the scanning speed, or the accessory installations and options. Additionally, the behavior of the instruments, e.g. the instrument live display under PC control, is different.

The following instruments are compatible:

- Thermo Scientific GENESYS 10 Vis, Bio, UV/Vis, BioMate 3S and Evolution 60S (not GENESYS 20)
- Thermo Scientific Evolution 200 series
- Thermo Scientific Evolution 300

Note: *With spectrometer models with limited wavelength range or if a required accessory (esp. integrating sphere) is not applicable, some of the parameter offered by the software cannot be executed.*

The following accessories can be attached (where applicable). They are automatically detected:

- Cell changer
- Sipper accessory (specific instruments only)

- External PC-controlled sipper pump (Economy Sipper)
- Peltier Temperatur Controller

Optical accessories like specular reflectance attachment, integrating sphere or micro illumination are not specifically detected by the software.

The software anticipates these details as far as possible. A description of the various instruments details is given in: *Spectrometer and Accessories* 10-1. Please read this information before starting your first measurements.

2.3 Installing the Software

In order to install the software you must be logged on as the administrator.

Note: *For a USB interfaced spectrophotometer and/or Peltier accessory, the device should not be powered.*

Note: *When the software will be installed with **VISIONlite**, it should be installed after that. Thus, the same program and data directory is offered. These settings assure that VISIONlite ColorCalc shares the same directories and that it is entered to the VISIONlite start routine. See also below.*

Note: *The optional additional **Reporter-SPX** software should be installed after **VISIONlite ColorCalc**.*
***Tip**: For reviewing or learning the software operation, the software can also be installed in the demo mode. In this mode all functions are available, and data recording is simulated with synthetic data. Instrument parameters are generalized. Loading spectrum files is restricted to the file **demo.dsp** as supplied with the installation.*

Executing the Software Installation

First, close all other active applications. Normally the installation routine starts automatically when you insert the software CD into the appropriate drive. If it does not start, please start the **setup.exe** routine in the main CD directory.

In Windows Vista/7/8/8.1 the privilege elevation (UAC) message will appear:
An unidentified program wants access to your computer.
or
Do you want to allow the following program from an unknown publisher to make changes to this computer?

Select **Allow / Yes** to continue.

Thereafter, the installation routine will guide you through the installation procedure. The following steps are performed. Make your choice(s) and accept the entries via the **OK** button. The **Exit Setup** button allows cancelling the installation process in each step.

1. You are reminded to close all running applications. Exit the installation if this is not yet the case. Thereafter, close all other software applications, and start the installation routine again.

2. Enter the 12-digit software serial number. The serial number is printed inside of the cover sheet of the printed manual. Alternatively you can also install the software in a demo mode: For an installation in demo mode, select **demo mode** without entering the serial number.

3. According to Windows conventions the software installs to the Program directory
   C:\Program Files\VL_ColorCalc
   (Local language Windows Vista/7 installations may use the translated designation of Program Files). This directory is shown as the default installation directory.
   If an existing installation of the Thermo Scientific **VISION*lite*** software is detected, the respective program directory is shown.
   Use the **Change directory** button to choose a different directory or to define a new directory, if required.

4. In the next window select your language of choice as the software language.

5. Thereafter select your type of spectrophotometer or group of spectrophotometers (not for an offline version). See also: *Starting the Software* 3-1.
   RS-232 interface only: In the next window, select the interface used to connect the spectrophotometer to the PC. This is typically **COM 1**. The setting can also be changed later on during software operation.

6. The software is usually installed in its own program group. Optionally, you can select a different program group or define a new one.

7. For further files and for the methods and results subdirectories, the Data directory use the path
   C:\Users\Public\(Public)Documents\VL_ColorCalc
   is applied with Windows Vista/7/8. Local language Windows installations may use translated designations.
   For older Windows versions, the path
   C:\Documents and Settings\All Users\(Shared)Documents\VL_ColorCalc
   is used.
   Use the **Change directory** button to choose a different directory or to define a new directory, if required.
   Automatically the **Results** and the **Methods** directories are generated as subdirectories of the Data directory.

8. After the queries, the setup routine initiates data transfer from the CD to the hard disk. For spectrophotometers with USB port, a USB driver is installed: The message
   Would you like to install this device software
   is given. As the publisher *Thermo Scientific* is named. Accept the installation by clicking **Install**.
   The same applies for the Peltier accessory. For this select the port after installation in the **Options/Preferences/Spectrometer** function.
   The driver is set up automatically, when the instrument is connected and powered first time. The **Device Manager** then shows an additional port with the designation **Spectrophotometer / TempControl**.

Note: *If the software has already been installed previously or a software update is being done, the system will overwrite without query all files, which are of the same or a previous date as those of the new installation. Modified files can be preserved. See: Updating* 2-5

9. At the end of the installation you are asked if you want to see the **readme** file. This text file includes the latest information not yet published in this guide. Close the Notepad window after reading.

Implementation to the VISION*lite* Start Routine

When the software is co-installed to **VISION*lite***, it also automatically adds its entry to the startup routine of the **VISION*lite*** version 4.1 or higher software.

For previous versions, the **VISION*lite*** ascapp.cfg can be extended manually. See the respective software manual.
The *VL_ColorCalc.cfg* configuration file then must be extended with the definition of a start module. See *General and User Configuration File* 8-2.

Additional Licenses

If you want to use the software at multiple instances, you should purchase further licenses. If you want to use more than one instrument at one PC, you establish multiple installations. If so, make sure that you select a different interface, a different program and Data directory and a different program group.

Tip: *The second installation will overwrite the program icons on the desktop and the entry in the program group. Therefore rename the existing items beforehand.*

2.4 Configurations

- The software is designed to be run by a standard user without administrator rights. On systems with non-standards Windows access rights, it may be necessary to set the Read/ Write permissions manually.
- If you are also using the Thermo Scientific VISION*lite*® software, and you would like to share the results directories, re-define the directory path via the Options/Preferences software function. See Preferences 5-12.
- For reflectance measurements, the required white and dark correction data files should be adapted to the specifics of the measurement system, see Reflectance Measurements 8-9.
- If additional information is to be placed in the title bar of the main software window, e.g. the instrument identification number, this information is added to the program start line, see Options in the Software Start Line 8-7.
- A call of the software can be extended by adding the name of a method, which is to be started with the software. Further definitions are possible. Thus, the desktop may include several icons for different standard procedures, see Options in the Software Start Line 8-7.
- Further configurations options like import/export formats, print details or handling of sample names can be configured in configuration files, see Options in the Configuration File 8-3.

Offline Configuration

The software can also be operated in an offline mode. This is done either via installation with an appropriate serial number or by setting the spectrometer port to **<None>**. See *Options menu/ Preferences* 5-12.

2.5 Updating

The software is regularly improved and and extended, which results in releasing new software versions. Updates can be installed with the existing software serial number. This section provides information for users who already have been working with former software versions. A version history of this software is contained in the CD's *manual* directory.

Note: *During installation of a new version in the place of the old version, the user is queried to overwrite existing files which have been modified. Make sure you keep important data.*

When updating an existing software version to a newer version or re-installing, you may select the existing directory structure in the setup procedure. In this case, the installation will overwrite without query all files, which are older than those of the new installation or which have the same date and time of generation. User created files like spectra or methods will remain intact. Files, which have been modified in previous use, for example the initialization file, the parameter definition file or the default method files, will be newer than those on the installation disk. In this case you are queried if you wish to keep these files. Select **No to all**, if you wish to have a completely new installation.

Alternatively, also a different Program and Data directory can be selected. Thus the original installation will remain intact. Then, also select a different name for the program group. If this new name includes the name of the original installation, this name will also automatically be applied for the new desktop icon and the program group entry. Else, you should rename the existing program group and desktop icon of the initial installation so that they are not overwritten by the new installation.

When updating from **VISION*lite* ColorCalc**, take note of the changes to the software organization and formats, described in the following sections. For existing methods, new instrument parameters are set to defaults, so that also existing methods can be used with the new software version.

Software Organization

A number of files that have been located in the Program or the ProgramData directory in previous versions, are installed in the *Public,* resp. *All Users* directory, i.e. typically

C:\Users\Public\(Public)Documents\VL_ColorCalc (Windows Vista/7/8) or
C:\Documents and Settings\All Users\(Shared)Documents\VL_ColorCalc (Windows XP).

This is done according Microsoft recommendations. The contained files include the configuration file and the *Results* and *Methods* directory, see below.

Results and Methods Directory

When updating from **VISION*lite* ColorCalc** version < 2.0 also observe the modified default setting and naming of the results and methods directory. The data directory has been renamed to **Results**. It is located in the **Data** directory just as the **Methods** directory. Modify the settings after installation, if you want to retain the old structure or transfer your relevant results and methods accordingly. See: *Methods* 4-1.

Configuration Files

Compared to **VISION*lite* ColorCalc** version < 2.0, the configuration file has been split into 3 files

and the the syntax has been changed. Therefore, the existing software configuration file of a previous version cannot be maintained. Special software configurations must be redefined with the new structure and syntax after the update. See: *Software Configuration* 8-1.

Parameter Definition File

Note that for the parameter definition file, the syntax has been changed essentially with **VISION *lite* ColorCalc** version 5.2. Existing methods must be redefined in terms of the selection of evaluations. Modifications of the existing parameter definition file must be redone. See: *Adapting Calculation Parameters* 8-17.

Results and Methods

Newer versions will be able to read and load existing spectra. If the newer version handles additional spectrum parameters, spectra of the older version receive a default entry for these parameters.

With newer versions, generally, the list of calculation parameters has been extended and modified, see also above. Therefore, it will be necessary to update the **Calculations** definitions of existing methods:

1. Load the method and open the **Calculations** window.
2. Redefine the required calculation parameters.
3. Store the method.

Note: *Also, some parameter designations might have been changed e.g. due to revised versions of the underlying norms.*

Change of Spectrophotometer

Also, the software can be continued to be used with a change of instrument. Generally a software re-installation is required. If the instrument is of the same group, e.g. Thermo Scientific GENESYS S series, this is not required. It may be necessary, to redefine the instrument method parameters.

3 Starting the Software

Before you start the software, look up the information about your specific instrument. Some models, for example, must be switched to remote control. See: *Spectrometer and Accessories* 10-1.

The software can be started either from the program group

or with the respective icon on the Windows desktop. 

If the software has been co-installed with **VISION*lite***, the software can also be started from the **VISION*lite*** start routine; see the respective manual.

When started, the software takes up the current instrument settings and activates the Live Display, if the connection has been established successfully. When the spectrophotometer is still initializing, an appropriate message will be issued. If the communication cannot be established, the software displays the respective error message and the Live Display remains inactive. After accepting this error message however, offline data and method handling is possible. See: *Offline Operation* 8-1.

***Tip**: Please note that some spectrophotometer models like the Thermo Scientific Evolution 600 may require several minutes to establish PC-control.*

After installing or removing an accessory or after modifying the communication configuration or the parameter definition file, it is necessary to restart the software so that the new configuration is detected.

Use the **Optical Alignment** command (specific instruments only) to align the position of micro cells or an accessory like the integrating sphere. See: *Optical Alignment* 5-11.

Alternative Start Methods

The software can alternatively be started with a dedicated start line. This can be a definition of a desktop icon or a start from another software. See section *Options in the Software Start Line* 8-7.

Also, the software can be started by clicking a linked method or spectrum file. The file types are linked with the software installation.

A configuration option defines the handling of multiple software starts. See section *Options in the Configuration File* 8-3.

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4 Overview

The software is designed to record a sample spectrum and to evaluate the spectrum with the selected calculations. See: *Calculations Window* 5-21.
Spectra can be reloaded and re-evaluated.

After installation and setting up some essential configuration parameters (see: *Software Configuration* 8-1), you operate the software mostly through its main window. See: *Software Operation* 5-1.

The main window provides all operating functions:

- Defining methods
  All measurement and evaluation parameters are summarized in a method, which can be easily employed for routine operation. The name of the current method is shown in the methods selection field at the top of the parameter area. See: below and *Method list box* 5-15.
- Selection of required evaluation parameters in the **Calculations** sub window, see: *Evaluation Parameters* 7-1.
- Scanning sample spectra, see: *Measurement* 6-1.
- Offline evaluation of spectra, see: *Recalculation* 5-33.
- Presentation of spectrum graph(s) and calculation results, see: *Graph Area* 5-26 and *Results Area* 5-32.

Based on the existing calculation option, the evaluation parameters can be modified and further evaluations can be added, see *Adapting the Evaluation Parameters* 8-17.

Tip: *A spectrum demo.dsp is installed to the results directory by default to allow first steps without an instrument.*

Methods

Methods are parameter files that include data recording, data evaluation and result output settings. Method files are characterized by the file extension **mol**. With this option you can save and restore standard parameter settings for routine measurements.

When the software is used for the first time, the basic method *test1* is opened. You can modify the settings of the basic method and you can save these settings as the modified basic method. You can also generate further methods under new method names. To save a method you use the **Save Method** command in the **File** menu. See: *File Menu* 5-3.

Tip: *Methods can only be saved, when the software communicates with the instrument.*

You may recall existing methods in 2 ways:

- Select a method in the **Method** list box in the parameter area. The **Method** list box lists all methods of the current method directory. See: *Method list box* 5-15.
- Click the **Open Method** command in the **File** menu. See: *File Menu* 5-3.

Settings of a method can no longer be altered when the write-protected attribute has been given to the method file via the Windows Explorer, see *Protected Methods* 8-12.

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5 Software Operation

You operate the software mostly through its main window that features several standard Windows elements for operation:

- Title bar, holding the name of the software and, if implemented, an additional label defined by the customer. See: *Software Configuration* 8-1.
- Menu bar and tool bar with buttons and live display. See: *Operating Toolbar* 5-2.

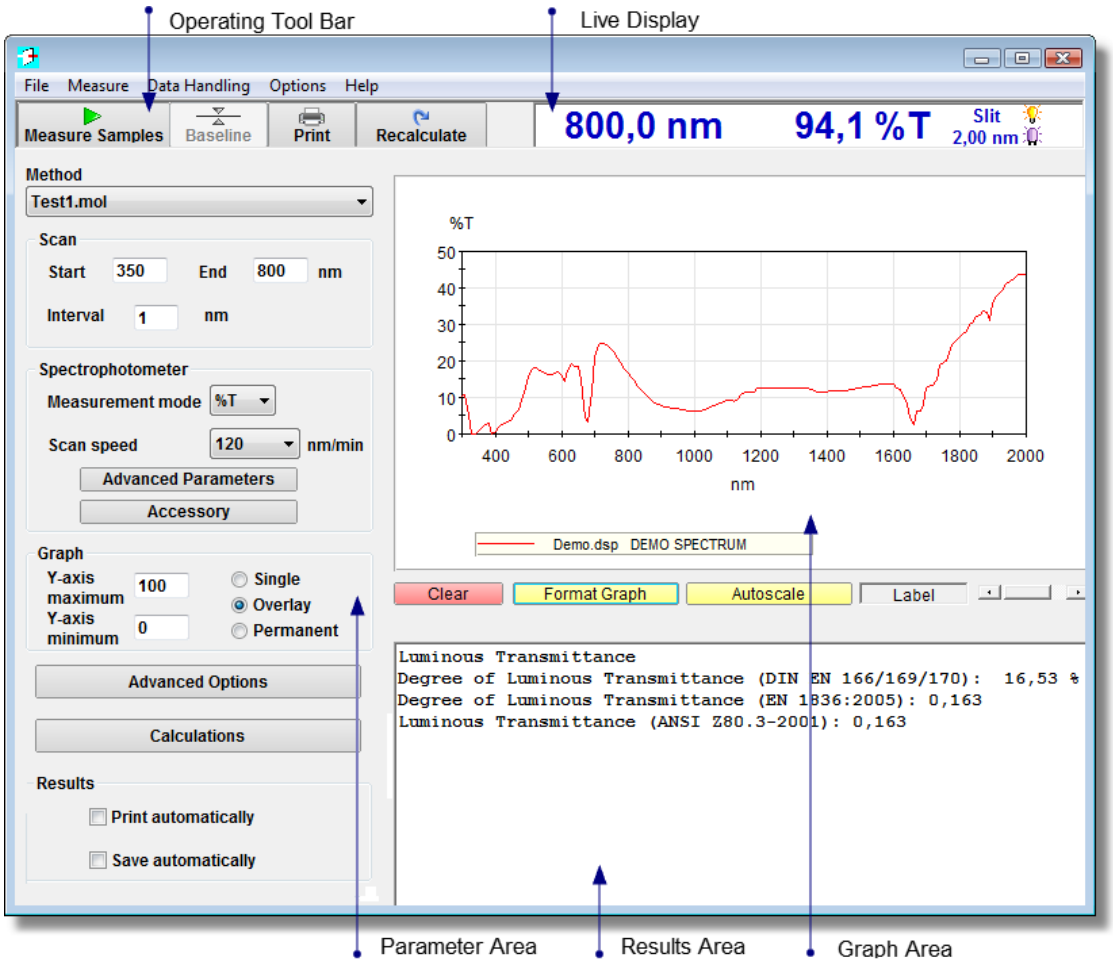


Figure: Main software window

Below this the main program window is divided vertically into two halves:

- The parameter area on the left side of the window presents all settings and options for measurement and evaluation. Depending on the specific parameters, selection boxes, entry fields or selection buttons are available. See: *Parameter Area* 5-15.

Note: *If the software is configured to offline operation, these options are not shown.*

- The right window section is reserved for the output of results. The upper graph space displays the scanned spectra graphically. Buttons are available to modify the graph. Alphanumerical results are displayed in the results space below the graph. See: *Graph Area*

5-26 and *Results Area* 5-32.

Use the upper results space border to resize the areas via drag and drop with the mouse.

5.1 Operating Toolbar

The operating toolbar below the menu bar contains buttons to operate the basic measurement and the data evaluation functions.

Table: Buttons of the operating toolbar

Button	Function
Measure Samples	Start of a series of measurements. See: *Measurement* 6-1. ***Note:*** *Not shown or deactivated in offline mode.*
Baseline	Start of a baseline compensation run. ***Note:*** *Not shown or deactivated in offline mode.* ***Note:*** *With a sipper, the background sample is not aspirated.*
Print	Printout of the report without opening the printer setup window. See: *Print Commands* 5-5.
Recalculate	Start of a recalculation of results for the displayed spectra. See: *Recalculation* 5-33.

The buttons can change their designations, depending on their current function, e.g. the change from **Measure Samples** to flashing **Stop** button. Grayed-out buttons are inactive at the time.

Figure: The operating toolbar

Live Display

A live display appears at the right-hand side of the toolbar. The live display continuously displays the current wavelength and ordinate (not possible for some models; solely with restrictions during autozero/baseline measurements).

The live display shows ***-.- nm***, if no instrument is connected. It shows **********, if the instrument is not powered, or the lamp has failed or is switched off in standby or if the software is in offline mode.

Note: *Ordinate readings can be erroneous if no autozero / background correction exists for the current wavelength. See: Measurement* 6-1.

Note: *When the **%R** or the **f(R)** ordinate mode is active, the Live Display shows reflection corrected ordinate values.* See: *Reflectance Measurements* 8-9.

The live display also depicts the current **Slit** setting (spectrophotometers with adjustable slit widths) and the current position of the cell changer, where applicable. For instruments incorporating continuous light sources (not pulsed Xenon sources), the on/off status of the lamp (s) is shown as a pictogram. Further instrument/accessory parameters are shown if applicable.

5.2 File Menu

The **File** menu contains commands for data handling and output:

- **Open / Save Method**
- **Show Method**
- **Load Spectrum / >>> / Save Spectrum as**
- **Export Results**
- **Export** – only with additionally installed **Reporter-SPX** software
- Print commands: **Print**, **Print Preview**, and **Printer Setup**
- **Change Application** – only if software is co-installed with VISION*lite*. See *Software Installation* 2-2.
- **Exit**

The commands are described below.

Open Method Command

The **Open Method** command presents a window listing all methods (extension .**mol**) in the currently selected method directory. The method directory is defined in the **Options/ Preferences** command. See: *Preferences* 5-12. A different directory can also chosen. Select the requested method file and confirm by clicking on the **Open** button. The method settings are assigned to the various parameters.

It is also possible to load a spectrum as a method file: in the **Open** window, switch to the Results directory, enter ***.dsp** and click **Open**. Select a spectrum file from the list. As far as possible, the method parameters are taken from the file; not however the calculation parameters.

Alternately you may select a method from the **Method** list box in the parameter area. See: *Method list box* 5-15.

Save Method Command

The **Save Method** command is used to save the current measurement and evaluation parameters to disk as a method file. The method can be applied for later use of these parameters. The command opens a **File Save** window, where you enter the method filename. The appropriate method file extension is attached automatically. The current method directory is offered as the directory in which to save the method; however you can select different directories.

Note: *The **Save Method** command is inactive, as long as the software has not identified the attached spectrometer, e.g. if the instrument is switched off or disconnected.*

Show Method Command

The **Show Method** command opens a print preview window and presents the method settings and the audit trail information of the currently active method. The listing does not include the selected calculation parameters.

Load Spectrum Command

With the **Load Spectrum** command you load saved spectral files from disk to the graph. It is possible to inspect older data, to compare and to re-evaluate them with the **Recalculate** button. See: *Recalculation* 5-33. Up to 50 spectra can be loaded.

The command displays the **File Open** selection window, which lists all saved data of the respective type in the results directory. A different directory can be selected. Select the requested file or files (with [Shift] or [Ctrl] key) and confirm by clicking the **Open** button.

The function reads spectra, which have been recorded by **VISION*lite*** or **VISION*lite* MaterialsCalc** / **VISION*lite* ColorCalc**. Additionally, you can import other spectrum formats. See: *Data Formats and Import/Export* 9-1.

Tip: *In order to view only spectra of a selected file extension, type e.g.* ****.dx*** *and press [ENTER]. Accordingly, the entry* ****.**** *lists all spectra of the selected folder. With the file extension <.sp> binary UVWinLab (2.0-3.0) and PECSS/PECOL spectra can be loaded, with the extension <.asc> UVWinLab spectra in the ASCII format can be loaded.*

Recently used Files

The command **>>>** shown below **Load Spectrum** opens a list of names of the up to 9 recently used (measured or loaded) spectra from the results directory. By clicking on an entry, the file is immediately loaded.

The list is handled in the user-specific configuration file so that it is specific for the user that is currently logged in at Windows.

Tip: *After a change of the results directory path, listed files will no longer be accessible by this functions.*

Save Spectrum as Command

With the **Save Spectrum** command you save spectra to disk. This command displays the **File Save** window for saving the spectra with the extensions **.dsp**. Additionally the file formats **csv** and **JCAMP-DX** are available.

All spectra present in the graph will be presented for storage. A different name and directory can be selected. As a default, the currently active results directory is shown. See: *Preferences* 5-12.

Tip: *Spectra are stored to disk automatically after recording. The* ***Save Spectrum*** *command is mainly used to store data with a different name and directory.*
Tip: *The* ***Spectrum*** *Information window offers an option to save single spectra.* *See: Spectrum information window* 5-30.

Export Results Command

This command allows the results to be saved to disk as a **.csv** file (comma separated values). See: *Data Formats and Import/Export* 9-4. The files contain all results in a tabular form. As a filename, the name of the (first) spectrum is offered. The files can be read by spreadsheet programs like Microsoft Office Excel.

Tip: As an alternative to this option, an additional function can be implemented to copy the results to the clipboard. *See section Data Handling and Utility Templates* 8-12.

*Tip: Spectra can be exported in tabular form as .csv files via the **Save Spectrum as ...** command. See above.*

Export Command

The **Export** command is only available with additionally installed **Reporter-SPX** software.

The command stores a report of the current measurements in a selectable format. See: *Report Configuration* 8-35 and the *Reporter-SPX Operator's Manual*.

Print Commands

The **Print** command prints the current report. You can select the printer, the number of copies, etc. in the print window. Additionally you can set the printer attributes. See also: *Preferences* 5-12.

The **Print Preview** command opens a **Print preview** window, which shows a preview of the printed report. In this window you can swap pages, modify the size of the presentation, and actuate the printout. Close the **Print preview** window to return to the software operation. See: *Print Preview* 5-6.

The main function of the **Printer Setup** command is to select a printer. You also can preset various printer settings. The possible options are determined by the printer driver.

***Tip:** Several printer drivers do not accept these settings. In this case, use the printer driver to define printers settings.*

Change Application Command

The command is only available, if the software is co-installed with the Thermo Scientific VISION *lite* software. See *Installation Procedure* 2-2.

The command closes the software and returns to the VISION*lite* start routine. This allows a quick change to another application of the VISION*lite* software.

Exit Command

The **Exit** command closes the software. If you have modified any parameters of the current method you are asked whether you wish to save these changes.

5.2.1 Print Preview

The **Print Preview** command opens a print preview window, which shows a preview of the report. In this window you can swap pages, modify the size of the presentation, copy it or actuate the printout.

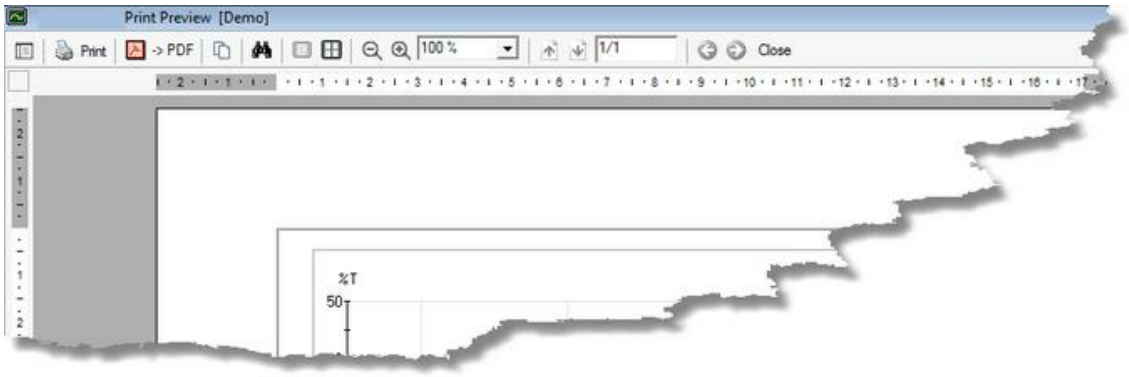


*Figure: The **Print Preview** window*

The header title in the **Print Preview** window displays the name of the evaluated spectrum, or the name of the first spectrum of a series of spectra, respectively. The functions are available in a toolbar.

*Table: Commands in the **Print Preview** window (from left to right)*

Command	Function
Contents	Opens a column at the left-hand side of the screen to show report contents. This option is not used.
Print	Initiates the printout of the current report.
-> PDF (Export To PDF)	Stores a report file in the PDF format. The filename is equivalent to the sample name of the first spectrum/data set, or the results filename, respectively. When the *PDF_DirSelect* parameter is set in the configuration file, an additional **File Save** dialog allows entering a file name and storage path. ***Note:*** *There might be problems with this function with software installations in Korean or Chinese language.*
Copy	Copies the currently displayed page of the report to the clipboard.
Find	Opens the **Find** dialog that allows you to search for specific words or phrases in the report. Enter the search text to the **Find what** box in the **Find** window.
Single Page/ Multiple Pages	These buttons allow changing between a single page presentation and a multiple page presentation. When you select **Multiple Pages** additional buttons are presented to select the number of pages to be displayed.
Zoom Out/Zoom In	These buttons allow changinge the scale of the presentation. The selected scale is displayed in the selection box. Alternatively, in the selection box, you can also select a value directly or enter a new value.

Command	Function
Previous Page/ Next Page	If there is more than one page in the report, you can jump from page to page with these buttons. The page being displayed is shown in the text box. You can also enter a page number directly into the text box.
Move Backward/ Forward	These buttons are only active if there is more than one page in the report and you have already jumped pages. These buttons jump directly to the previously viewed page or back, respectively.
Close	Closes the **Print Preview** window to return to the main software.

5.3 Measure Menu

Note: *If configured to offline operation, this menu is not shown or it is deactivated.*

The commands of the **Measure** menu are equivalent to the buttons on the toolbar:

Samples The command starts a measurement series and is equivalent to the **Measure Samples** button. See: *Measurement* 6-1 and *Operating Toolbar* 5-2.

Baseline The command starts a background correction and is equivalent to the **Baseline** button. See: *Measurement* 6-1 and *Operating Toolbar* 5-2.

Note: *In cell changer mode, the blank sample for autozero/background correction must be supplied in cell position 1.*

Note: *In the sipper mode, the* **Baseline** *command does not aspirate a blank solution. Use the separate sipper keys or perform the autozero/background correction when running a method.*

Additional Commands

Further measurement functions can be added to the **Measure** menu via dedicated templates. See *Data Handling Templates* 8-12.

Function Keys

You can also activate the commands of the menu using a function key; the required function key is listed behind the command name. Using a function key is often more convenient while performing an analysis in the laboratory. The first 6 additional functions (see above) may be called by function keys F7-F12.

- **Samples / Stop** [F5]
- **Baseline** [F6]
- **Manual Control** [F4]
- **MethodLink** (see above) [F7]
- Additional measurement functions [F8-F12]

5.4 Data Handling Menu

The menu contains a number of simple, mathematical spectrum handling functions. These functions generally access the spectra that are currently shown in the graph area.

Additionally, functions are available to show the CIE 1931 color space chromaticity graph (xy horse shoe diagram) and CIE Lab* color difference graphics. For these, the respective results must have been generated, see below.

All these functions are based on **Reporter-SPX** template files with appropriate scripting functions that are resident in the Data directory. See *Report Configuration* 8-35 *and* the *Reporter-SPX Operator's Manual*.

Accordingly, the list of functions can be extended, eliminated or edited by the user. Further data handling functions are available in the software's /tools directory and can be activated. Overall, t he menu can hold up to 50 entries. If all functions are deleted, the Data Handling menu disappears. See *Data Handling Templates* 8-12.

Tip: *The functions are named with English designations which are derived from their filenames. By renaming a template file, a different naming also in your local language can be achieved.* See *Data Handling Templates* 8-12.

Data Handling Functions

Please note that the function designations are given in English but can be modified by the user. See *Data Handling Templates* 8-12.

The menu contains the following mathematical functions:

Command	Function
Add Value	Adds a user-entered numerical value to all spectra (max.10) of all ordinate modes in the graph. The result spectra are added to the graph with the name of the initial spectrum with an attached "_V". A remark is added to the spectrum descriptions. To subtract a number, use a negative value. This manipulation may not be meaningful for %T or %R spectra.
Adjust Abscissa	The function allows changing the abscissa start/end of the data and the data interval for all spectra displayed. When start/end values outside of the original data are selected, the spectrum is extended and the additional data points are set to zero. Thus it is possible to merge spectra by adding two spectra. If the data interval is selected smaller than with the original data, missing data points are linearly interpolated.
Derivative	Transforms all spectra displayed to its first, 2nd, 3rd or 4th derivative (D1-D4). A parabolic Golay-Savitzky smoothing algorithm is applied. For this, the calculation interval is selected as 5, 9, 21, 49 or 101 multiple of the spectrum data interval. The ordinate mode is changed to D1 - D4 accordingly (This is independent of the original ordinate mode.). Note that the spectrum range is reduced for half of the calculation interval at the low and the high end.
List	Opens the **Print Preview** window to list the spectrum currently present in the graph with all data points (according to its data interval). Only one spectrum must be present in the graph.
Mean	Calculates the average of all spectra, currently displayed in the graph. The

spectra must have the same wavelength range, ordinate mode and data interval. The result file is added to the graph as “mean.dsp”. The result file receives the description of the first spectrum; it is extended with a depiction of the calculation.

Merge

The function combines 2 spectra of the graph that have the same ordinate mode, but do not share the same wavelength range, to a new full spectrum. The result spectrum uses the lowest and the highest abscissa limits of the source spectra. In the range of overlap, the average of the spectra ordinate values is taken, in the range of a gap, ordinate values of zero are filled in. The filename and the file description of the result spectrum are put together from the sources.

Multiply Factor

Multiplies all spectra (max.10) in the graph with a user-entered value. The result spectra are added to the graph with the name of the initial spectrum with an attached “_F”. A remark is added to the spectrum descriptions. For a division, use the reciprocal as a factor.

PeakArea

The function allows calculating the area below the spectrum. Only a single spectrum must be displayed in the graph. The user is queried to select the start and end point of integration graphically: move the cursor to the required position and click. Note that the function is canceled, if the cursor is moved out of the graph. The area value is calculated as the area between the curve and the connecting line as a baseline within the selected interval. The result is placed in the result area.

Smooth

Applies a smooth calculation to the spectra displayed. This allows removing excessive random noise while largely maintaining spectrum details. The routine operates differently for a single spectrum or with multiple spectra.
In a first step it is queried, if the spectrum shall be smoothed over the full wavelength range or if a sub section shall be defined interactively. For that click the **Change** button.
A parabolic Golay-Savitzky algorithm is applied. For this, in a second step the calculation interval is selected as 5, 9, 21, 49 or 101 multiples of the spectrum data interval. With a single spectrum, interactively test different intervals to optimize the remaining distortion of spectrum details. The smoothed spectrum is added to the graph as *<name_SM>.dsp*. Press **OK** to terminate the loop.
With multiple spectra, all spectra displayed are immediately manipulated after selection of the parameters. The spectra names remain unchanged. Towards the high and the low end of the data, the calculation interval (and thus the smooth effect) is successively reduced. This allows maintaining the full spectrum range, but may cause minor artefacts.

Spectra Addition

Adds the first 2 spectra in the graph. A result spectrum is added to the graph with the name of the first spectrum with an attached “_A” and with a wavelength range of the overlapping range of the spectra. Ordinate mode and data interval are taken from the first spectrum. The result spectrum description is extended with a depiction of the calculation.
Note: Adding spectra with different ordinate modes or in %T/%R modes is possible, but may be physically meaningless.

Spectra Division

Divides the first spectrum in the graph by the second spectrum. The spectra must have the ordinate mode %T or %R. A result spectrum is added to the graph of the name of the first spectrum with an attached “_D” and with a wavelength range of the overlapping range of the spectra. Ordinate mode and data interval are taken from the first spectrum. The result spectrum description is extended with a depiction of the calculation.

Spectra

Multiplies the first 2 spectra in the graph. The spectra must have the

Multi-plication	ordinate mode %T or %R. A result spectrum is added to the graph of the name of the first spectrum with an attached "_M" and with a wavelength range of the overlapping range of the spectra. Ordinate mode and data interval are taken from the first spectrum. The result spectrum description is extended with a depiction of the calculation.
Spectra Subtraction	Subtracts the second spectrum in the graph from the first. The result spectrum is added to the graph with the name of the first spectrum with an attached "_S" and with a wavelength range of the overlapping range of the spectra. Ordinate mode and data interval are taken from the first spectrum. The result spectrum description is extended with a depiction of the calculation. **Note:** Adding spectra with different ordinate modes or in %T/%R modes is possible, but may be physically meaningless.

Note that resulting spectra are not stored automatically. Use the **Save Spectrum** function to permanently store the spectra.

CIE 1931 Color Graph

The function **Color Graph CIE 1931** presents a color graph that depicts the measured sample's colors as marks within the graph. Thus the graph allows checking the sample color visually. See *Colorimetric Evaluations* 7-5.

Note: *The graph is only generated, if a xyY calculation has been done and the results are presented in the results area. If several xyY calculations have been selected for a sample, results of the first xyY calculation are applied.*

Note: *Technically speaking the graph is only valid for CIE 1931 (2 deg observer) calculations. However, deviations typically are small.*

Color Difference Graph

The functions **Color Difference Graph_L5_ab5** and **Color Difference Graph_L15_ab15** generate a report that show the calculated CIE Lab* color difference values graphically. The graph scaling is defined by the attached numbers and can be modified. See *Color Difference* 7-8.

Note: *The color difference graph is only generated, if a CIE Lab* color difference calculation has been done and the results are presented in the results area. If several CIE Lab* color difference calculations have been selected for a sample, results of the first calculation are applied.*

5.5 Options Menu

The Options menu includes the following commands:

Preferences Command

You use the **Preferences** command to define basic settings of the software, the spectrophotometer and printing. The settings are grouped through parameter groups found on the following tabs.

Group	Settings
General	On this tab you select the **data** and **method** directories.
Spectro-photometer	On this tab you define special settings for the instrument. See: *Spectrometer and Accessories* 10-1.
Printing	On this tab you define printing parameters, such as print color and line thickness.

For more information refer to the section *Preferences* 5-12.

Manual Control

This command opens the **Manual Control** window. It allows you to select instrument settings. Ordinate values can be read from the Live Display. (See: *Operating Toolbar* 5-2) You cannot perform any further measurements, evaluations or printouts via this command. See: *Manual Control* 5-13.

Optical Alignment Command

This command is only available with specific instruments. See: *Spectrometer and Accessories* 10-1.

The **Optical Alignment** command is applied to align micro cells or accessories like the integrating spheres in the light beam of spectrometer. See *Optical Alignment* 5-14.

Page Designer

The **Page Designer** command is only available, if the additional **Reporter-SPX** software is installed.

The command starts the software module for configuring the page layout of the reports.
For detailed instructions on the **Reporter-SPX** software, see: *Report Configuration* 8-35 and *Reporter-SPX Operator's Manual*.
A brief description of the **Page Designer** options is given in the section *Page Layout* 8-39.

5.5.1 Preferences

You use the **Preferences** command to define basic settings of the software (**General**), of the **Spectrophotometer** and for **Printing**. The settings are grouped through tabs.

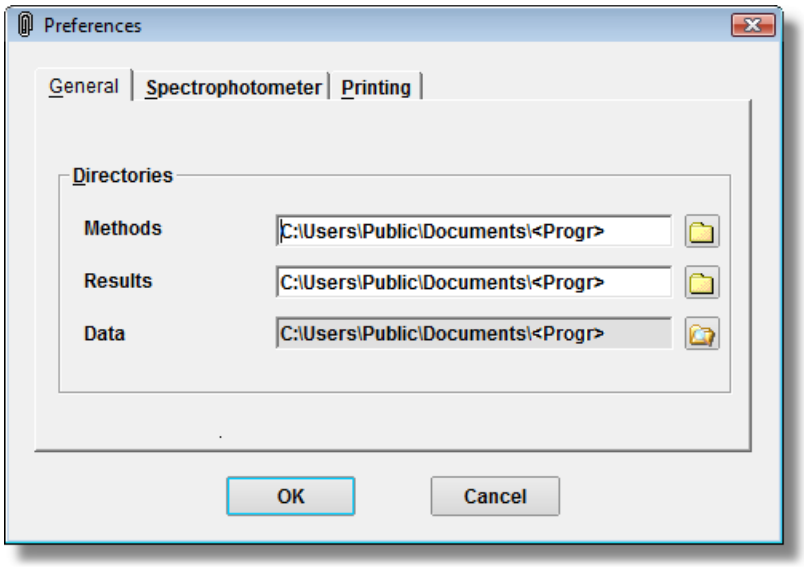


Figure: The Preferences window/General tab
<Progr> = program name
(Spectrometer tab not present in offline installation)

General Tab

The **General** tab allows you to select the results and method directories. The software saves data/results and methods in two different directories, which can be located at any position in the directory tree. You can directly edit the directory names or ...

1. Open the directory selection window with the directory symbol following the entry field.
2. Double-click on the required directory or define a new directory.
3. Confirm your selection by clicking the **OK** button.

Also, the tab displays the path of the **Program data** directory. This directory contains a number of configuration files, such as the reflectance correction spectra files or the configuration file. The path cannot be modified.

Clicking the button behind the text field opens the Windows Explorer with the **Data** directory active. Use the Windows Explorer to edit, rename or move files of this directory.

Spectrophotometer Tab

The **Spectrophotometer** tab allows you to define special settings for the instrument. In particular in the **Spectrophotometer port** selection box you can select the COM interface of the PC (**COM1** to **COM64**), to which the instrument is attached. With a USB connected instrument, the port designation is shown, but cannot be switched to another port.

Note: *If you change the COM interface without correspondingly changing the socket into which the cable is inserted, communication between the PC and the spectrometer will be interrupted.*

Besides the numbered ports it is also possible to select **<None>** as the first entry of the selection list. This setting is used for offline operation of the software. Most instrument related functions are removed and the software will not try to communicate with the instrument. A changed setting only becomes valid next time you start the application.

When the Peltier accessory and/or the autosampler are attached to the PC, an equivalent COM selection box is shown for these devices.

Other settings depend on the instrument used, e.g. the selection of the Auto-3/Auto-6 cell changer mode. For details see: *Spectrometer and Accessories* 10-1.

Printing Tab

The **Printing** tab allows you to define printing parameters, such as the print color and line thickness.

The **Printing Mode** defines if the graph printout is in color or in black. The default **Automatic** setting applies the attributes currently selected for the printer. The **Color** and **Black** settings override the printer settings. The **Black** setting transforms the colors of the curves to different dashed lines and shades respectively and only prints in black.

Tip: *In the configuration file the line thickness of the graph can be modified to narrow lines (parameter **PrintMetaFile**). The setting is especially valuable for printing graphs with multiple spectra. Please note that due to the different transfer of graphic data details of the graphics printout may be changed. See: Software configuration* 8-1.

It can also be selected to have a presentation of print pages in **Portrait** (default) or in **Landscape** format. Printing in landscape format applies an alternative default print template. See *Report Configuration* 8-35.

The **Font Size** parameter selects the font size of the standard text output of a report. The default setting is 9.

The default entry of the **Footnote** parameter field is the software designation. To define different footnote contents, enter the text into the **Footnote** parameter field. This text is printed with the current date and time on the left and the page designation *Page n of m* on the right side in the bottom line of each report page.

5.5.2 Manual Control

This command allows you to select instrument settings without starting a measurement; e.g., to drive the instrument to a specific wavelength or to autozero at the selected wavelength. Ordinate values can be read from the Live Display. You cannot perform any further measurements, evaluations or printouts via this command.

Tip: *The function may also be initiated with the [F4] function key.*

You can:

- Drive the instrument to a specific wavelength,
  Tip: *If the instrument allows the option, also negative wavelengths below 0 nm can be entered. This allows checking wavelengths around the "white light" position.*

- Perform an **Autozero** at the selected wavelength (see: *Spectrometer and Accessories* 10-1), Switch the lamps: **UV lamp and Vis lamp** on/off (spectrometers with continuous radiation sources).

- Select the **Slit** setting (spectrometers with variable slit).

- If an accessory is attached, the control options of this accessory are additionally presented, e.g. driving the cell changer to a required location or actuating the sipper pump.

The spectrophotometer will immediately execute a choice from a list or a click at a button. Numerical entries like the wavelength setting are actuated with the **Apply** or **OK** button. The **OK** button also closes the window.

Accessories

If a sipper or a cell changer accessory is attached, the control options of this accessory are additionally presented, e.g. driving the cell changer to a required **Cell** position or actuating the sipper pump.

Note: *In the cell changer mode, the blank for autozero/background correction must be supplied in cell position 1.*

In the sipper mode the commands **Sip sample**, **Return sample** (some sipper models do not support this functions) and **Calibrate** (specific instruments only) are available. See *Sipper Accessory* 10-11.

Note: *In the sipper mode, a blank solution is not aspirated with the **Autozero** command. Use the separate sipper keys or perform the autozero/background correction when running a method.*

5.5.3 Optical Alignment

This command is only working with Thermo Scientific Evolution 300. See: *Spectrometer and Accessories* 10-1

The **Optical Alignment** command is applied to align micro cells or accessories like the integrating spheres in the light beam of spectrometer.

In a first step, the command requests, whether an integrating sphere is built-in in order to adapt parameters. The the command sends the instrument to a wavelength setting so that the beam in the sample compartment is visible to the human eye. Generally, this is “zero” nm. With this setting, the monochromator grating only acts as a mirror so that the measurement beam(s) are brightly visible for alignments.

The software then starts a time dependent measurement of the signal intensity and displays the readings graphically to allow the alignment. The user can cancel the command any time or it is automatically terminated after 5 min.

Note: *The background correction run must be repeated after an optical alignment has been performed.*

Tip: *The command is not available when the **Spectrophotometer port** has been set to **None**. See: Preferences* 5-12

5.6 Help Menu

The **Help** menu follows the standard Windows conventions.

- The **Contents** command opens a comprehensive help system. You operate this help system according to standard Windows conventions.

- The **Info** command provides information about the current software version and copyright.

Tip: *Also use the [F1] function key to open the help system with a page that corresponds to the currently active window.*

5.7 Parameter Area

In the Parameter area you select the method and the parameters to be employed for the sample measurement (scan) and evaluation/calculation. According to the parameter list boxes, buttons, sub-pages, etc. are used. An error message is displayed, if a parameter entry exceeds the allowed range.

Tip: *You can also use the tab key to change from one entry to another.*

At the top of the parameter area, the **Method** list box allows selecting the measurement method, see also section *Methods* 4-1.

The parameter area includes the following groups and buttons:

- **Scan**
  More information on performing measurements is given in the section *Measurement* 6-1.

- **Spectrophotometer** with **Advanced Parameters** and **Accessory** button (if applicable)
  For more information about parameters see section *Advanced Parameters Button* below.
  More information on parameters for accessories is given in section *Sipper Accessory* 10-1.

- **Graph**
  For more information on graphics see: *Graph Area* 5-26

- **Calculations** button; with this window you access the calculation parameters and the correction parameters for sample thickness. See: *Calculations Window* 5-21

- **Results**
  Information on the results display is given in the section: *Results Area* 5-32

Note: *If a method file has been assigned the read-only attribute, this is indicated by grayed parameter headings and by the message **Read-Only** (in red) above the **Method** list box. Thus you may protect methods against accidental or deliberate modifications. See: Protected Methods* 8-12

Note: *If the software is configured to offline mode (COM-port: None, see Preferences* 5-12*), the parameter area only shows the **Method** list box, the **Spectrum** list box (see below) and the **Calculations** button.*

Method List Box

The **Method** list box lists all methods files (file extension **mol**) of the current *Method* directory as defined in the **Preferences** command. Additionally, those methods are listed which were loaded

from other directories during the current working session. See: *Preferences* 5-12

Select a method by clicking on the name. All current parameter settings are changed accordingly.

Using the **Open Method** command will also allow you to access method files from other directories. After you have done so, the method is also listed in the **Method** list box during the current session. See: *File Menu* 5-3. With the next session, again only method files from the predefined method directory are listed.

Tip: *As well, you can modify individual parameters before the measurement. Use the* ***Save Method*** *command to create a new method after modifying an existing one.*

Spectrum List Box (offline mode only)

If the software is configured to offline mode, the operational elements listed below are not shown. Instead, the **Spectrum** list box is shown. This box is not available for normal operation.

The box lists all spectra that are available in the *Results* directory as defined in the **Preferences** command. The list is updated after 5 s interval time and if the software window is redrawn or the mouse is moved to another window element. Then the latest addition is highlighted. Thus, a spectrum file that has been generated by another software, can be easily loaded for evaluation.

Tip: *The update time interval is configurable. See the UpdateSpectrumList parameter: Options in the configuration file.* 8-3

Tip: *After clicking into the list, you may key in the filename of interest. The list will consecutively highlight the nearest hit. Thus extended scrolling of long spectrum lists can be avoided.*

Scan Group

The entry of **Start** and **End wavelengths** (nm) defines the spectral range to be scanned. The ordering is arbitrary. Make sure that the selected wavelength range covers the required wavelength range for the selected evaluation(s).

Note: *The wavelength range is automatically adjusted by the system, if the scan range is not a multiple of the data interval.*

Tip: *If technically feasible, entries around the wavelength "0 nm" can be selected to check the instrument white light alignment.*

Additionally you enter the **Interval** (nm) as the data point distance. The maximal entry is 10 nm; the minimal entry depends on the instrument model and the selected **Scan speed**. When the selected data interval is different to the definitions of the selected evaluation, the data are interpolated accordingly.

Note: *Make sure that the scanned wavelength range covers all wavelengths needed for the defined calculations. The interval is selectable since the data are interpolated according to the calculation requirements. However generally a data interval of 5 nm or smaller is recommended to achieve an acceptable accuracy of the results. See: Evaluation Parameters* 7-1

Additional specific parameters of the instrument may be shown. The layout and defaults of the

Spectrometer parameters depend on the associated spectrometer. See: *Spectrometer and Accessories* 10-1.

Spectrophotometer Group

In the **Measurement mode** selection box you select the measurement mode in which the data are recorded and presented:

Mode	Description
A	Absorbance / Optical Density Basically, all calculations available with the software are based on **%T** data. When **A** is selected as the data ordinate mode, the data are transferred to **%T** data for all standard color calculations. See the list of calculation parameters: *Evaluation Parameters* 7-1.
%T	% Transmittance
%R (*)	% Reflectance The **%R** mode is selected for reflection measurements using a dedicated spectrometer accessory, e.g. an integrating sphere. Selecting **%R** automatically employs the recalculation of the measured data with a white and a dark correction to generate absolute reflectance values. See: *Advanced Parameters Window* 5-19 and *Reflectance Measurements* 8-9. ***Note:*** *With reflectance measurement it is not feasible to define a path length correction. An error message is issued, when both settings are selected.*
f(R) (*)	Kubelka-Munk function The **f(R)** mode features a recalculation of the corrected % reflectance data according to the Kubelka-Munk function. The ordinate mode can be used for quantitative measurements of absorbing components in solid materials or powder mixtures. It is therefore sometimes called the absorbance for reflectance measurements. See textbooks on reflectance spectroscopy for further details. ***Note:*** *The Kubelka-Munk calculation uses white/dark corrected reflectance values. Make sure that proper reference spectra are defined.* ***Note:*** *For reflectance data over 100 %R, the Kubelka-Munk function generates positive values, similar to those shortly below 100 %R. For a differentiation, the f(R) values of readings > 100 %R are set negative. This is in analogy to absorbance data.*
SS, SR (only Evolution 200/300 series)	Single beam energy mode for sample (SS) and reference beam (SR)

*: not for GENESYS 10S series; otherwise only reasonable with reflectance accessory or integrating sphere installed.

Tip: *%R spectra can be transformed into the **Log 1/R** ordinate mode by applying the **A<>T** conversion in the **Spectrum** Information window. See: Spectrum Information window* 5-30

Other entry fields depend on the capabilities of the spectrophotometer, e.g. **Scan Speed**. Further settings are accessible with the **Advanced Parameters** button (see below).

Advanced Parameters Button

The **Advanced Parameters** button opens the **Advanced Parameters** window. This window allows you to select additional measurement parameters, which are less frequently used. The selected parameters are stored with the method. See *Advanced Parameter window* 5-19.

The button is inactive, if the instrument has not yet been identified, e.g. when it is switched off.

Accessory Button (only with accessory)

When a sipper and/or a temperature control is attached, an **Accessory** button is available to open the **Accessory** window. The window allows defining accessory parameters. The parameters are stored with the method. See *Accessory window* 5-20 *and Sipper Accessory* 10-1.

Graph Group

You define the initial graph scaling for the measurement via the **Y-axis minimum** and **Y-axis maximum** entry boxes. Selecting **0.00** for both parameters will generate a continuous (autorange) adaptation of the ordinate scale during measurement.

Tip: *Data exceeding the selected range are nevertheless recorded.*

During and after the measurement you can still modify the ordinate scaling.

The **Single**/**Overlay**/**Permanent** selection defines the graph overlay and the report generation:

Single	The graph is cleared with the measurement start and with each sample. The graph scaling is set up according to the method selection. A separate report is generated for each sample.
Overlay	The graph is cleared with the measurement start, but spectra within a series of samples are overlaid. The graph scaling is set up according to the method selection. A single report is generated for all measured samples, when the series of measurements is terminated.
Permanent	As above, but the graph is not cleared with the measurement start. Existing spectra and the graph scaling are maintained.

Tip: *By default up to 20 spectra can be overlaid. This figure can be modified by editing the configuration file.*

Advanced Options Button

The **Advanced Options** button opens the **Advanced Options** window that allows setting further measurement options. See: *Advanced Options* 5-21.

Calculations Button

The **Calculations** button opens the **Calculations** window. This window defines the parameters to be calculated from the spectrum and partially allows modifying them. Also the settings of the optional sample thickness transformation is accessible. See: *Calculations Window* 5-21.

Results Group

The **Autosave** and **Autoprint** selection buttons allow you to define the automatic handling of the results after measurements.

Note: *The **Autosave** and **Autoprint** settings are not valid for a re-calculation of results. See: Recalculation* 5-33

Selecting the **Autoprint** option will automatically print the results after measurement. The report consists of the spectral graph and the list of evaluation results. If the **Single** option has been selected in the **Graph** parameter group, printout takes place after each sample measurement. If the **Overlay** option has been selected, the spectra and results of a measurement series are summarized in a single report.

While scanned spectra are always saved automatically under the selected filename, the report is only saved automatically, if the **Autosave** option has been selected. The files are stored in the results directory with the filename automatically selected as the filename of the spectrum, or the first spectrum of a series. See: *Sample Information Window* 6-2

The report is saved in PDF format. By modifying the configuration file, it is possible to store the alphanumerical results alternatively as a text file (extension .txt). It is also possible to direct the report storage to a different directory than the results directory by modifying the configuration file. See: *Software Configuration* 8-1

If the configuration file specifies a directory for the report export or the PDF export, a csv- or a PDF-file is generated in this directory with the name of the spectrum or the name of the first spectrum of a spectrum series with the results of all spectra of that series. This is independent of the **Autosave** option. See: *Software Configuration* 8-1

Important: Reports are overwritten without query.

See also: *Results Area* 5-32

5.7.1 Advanced Parameters Window

The **Advanced Parameters** button opens the **Advanced Parameters** window. This window allows you to select additional parameters, which are less frequently used. The selected parameters are stored with the method.

- The **Reflectance Correction** selection box defines the set of reflectance correction data, which are applied for the reflectance measurements. This box is only active, if either the **%R** or the **f(R)** ordinate mode is selected. Select **Null**, if the readings are not to be corrected. The available correction data are typical materials absolute reflectance data, e.g. Spectralon ® and $BaSO_4$ (Barium sulfate/visible range). For precision measurement, you should adapt the correction data to your specific system. For more details see: *Reflectance Measurements* 8-9

- **Slit -** The **Slit** selection box defines the effective slit setting [nm] (only for spectrophotometers with adjustable slit widths).

Note: *For the model Evolution 220, the slit setting can also be adapted to the applied accessory e.g. with the settings **Sphere**, **Fiber** and **Micro**. See section Thermo Scientific Spectrophotometers* 10-1.

- **Lamp change -** The parameter sets the wavelength point of the lamp change. This parameter is only valid for instruments with two lamps.

Note: *Lamps (UV Lamp and Vis Lamp) can only be switched on/off via the **Options/Manual Control** command. The selected lamp will be not be included as a method parameter in the method file.*

Settings are stored with the method as a method parameter.

Press **OK** to accept the new entries.

5.7.2 Accessory Window

This window allows entering dedicated sipper, sipper/autosampler and external Peltier temperature control settings. It is not available for cell changer operation. Cell changer operation is not compatible with operation of a sipper. All entries in this window are saved with the method.

Sipper/External Sipper Pump

If a sipper or a PC-controlled external sipper pump (Economy Sipper) is attached, control options of the sipper are accessible via the additional **Accessory** button in the **Spectrophotometer** group. Click the **Accessory** button to display the **Accessory** window and set up the **Sampling time** (**Volume**), **Air gap, Waiting time** and **Reverse pump time** (only specific systems) for sipper operation.

The sample is aspirated for the selected **Sampling time**. Specific models alternatively offer a sample **Volume.** The volume is calibrated, see *Spectrometer and Accessories* 10-1.

Make sure to select a time/volume that sufficiently fills the flow cell without wasting sample and with a minimal carry-over from sample to sample. Depending on length and diameter of the tubing, type of flow cell and samples viscosity, a sample volume of a few milliliters should be sufficient.

Via the **Air gap** parameter, a small bubble of air is pumped after each sample to separate the samples and to generate a cleaning effect in the sample system. If an **Air gap** has been defined, the software gives an acoustic signal after the aspiration of the sample to make the operator remove the sample. After 2 seconds the sipper pump is started again to aspirate air. It is important that the volume is small enough so that no air will get into the cell.

The **Waiting time** is the time delay after aspiration and before the measurement. This parameter allows the sample liquid to settle and to remove streaks/schlieren, especially with long-path cells.

If **Reverse pumping** is available and defined, the sample can be regained after measurement.

Temperature Control

When the external Peltier Temperature Control device is connected to the PC and defined (see *Preferences* 5-12), the **Accessory** window offers additional parameters. To activate temperature control, select the **Active** switch.

The following settings are available:

Parameter	Function	Range
Temperature	Target temperature for the temperature-controlled cell holder	19 - 61 °C
Tolerance	Allowed tolerance of the temperature	0.1 – 9.9 °C
Stirring Speed	Speed of rotation of the magnetic field that drives the stir bar at the bottom of the cell	0 – 100 %

When the temperature control is activated, the start of measurement is delayed until the selected temperature (+/- tolerance) has been reached. The temperature will then be maintained constant during measurement.

Note: *Regard that the cell contents will have an additional temperature lag.*

5.7.3 Advanced Options Window

The **Advanced Options** button open the **Advanced Options** window. It allows you to define:

- **Start delay: Wait time** [seconds]
  This parameter is a time delay after starting the measurement by pressing the **Measure** button and before the actual start of data acquisition. The count-down of the delay time is shown in a separate window. Use this parameter for equilibration of the sample before the measurement.

- **Repetitive measurement**: **Total run time** and **Interval time**
  These settings reflect the timing for automatically repeated measurement cycles for repetitive sample measurement.
  The **Interval time** is the time delay between two subsequent scan starts [seconds]. The **Total run time** fixes the number of measurement cycles.
  You can deactivate this feature by setting the **Total run time** to '**0**' (zero).
  If the **Time interval** is selected shorter than feasible, the lowest possible time interval will be used automatically.

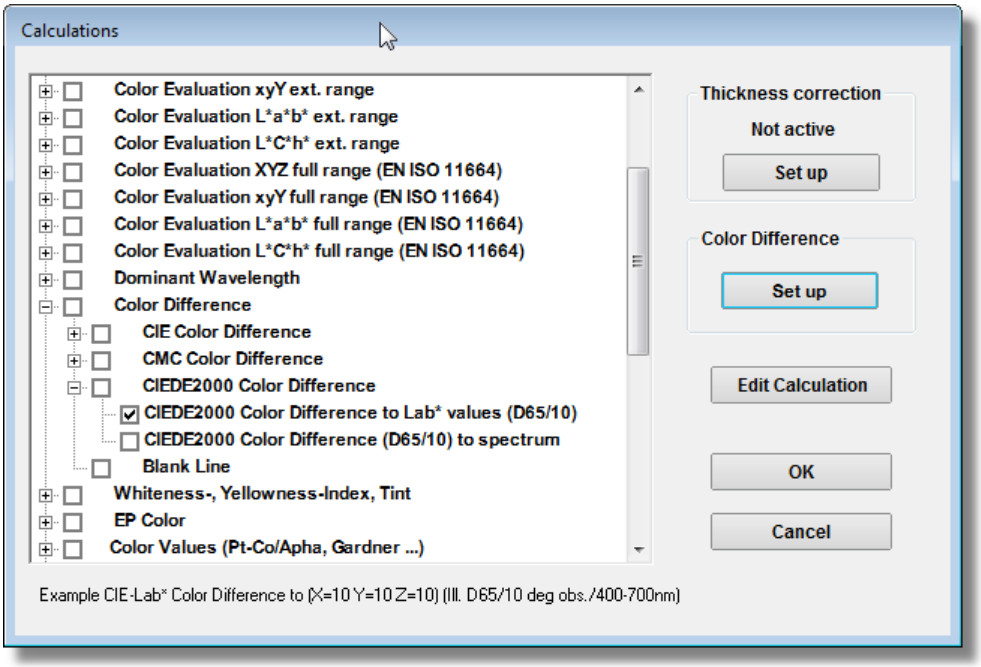
If a sipper is installed, the sipper can be defined to be actuated automatically with each cycle. See: *Accessory Window* 5-20.

Repetitive measurements can generate a large number of spectra. The filenames of the spectra series are generated by adding an incremented number to the selected filename: ***_001**, ***_002**, etc. The **Spectrum/Data** information window displays the number of the current cycle and, for replicates, the measurement time.

5.7.4 Calculations Window

The **Calculations** button opens the **Calculations** window. This window defines the parameters to be calculated from the sample spectrum/spectra and it allows opening the **Thickness correction** window and editing some of the parameter definitions, see below.

The selection list shows the list of available calculations. The list of calculations corresponds to the entries in the parameter definition file, see below. The calculations are presented as a short description name; a highlighted calculation parameter is described in more detail below the list. Select a required calculation parameter by clicking its check box. The selected calculations are integrated into the method. The results of calculations are output in the order as given in the list.



Calculations Window (Edit Calculation button see below)

Selecting the Required Calculations

1. In the main window click on the **Calculations** button so that the **Calculations** window opens.

2. The parameters list shows all calculation parameters as defined in the parameter definition file. Select any number of parameters.
   The available parameters are organized by sections in a tree structure. Use the **+** character to open the section and select specific parameters of the group or click the section box to select all parameters of the section. With a further click on the section box you clear all selected parameters of that section.

   Tip: You may structure the report output by selecting the section headings and empty lines.

3. Click on **OK** to confirm your choice or **Cancel** to exit the window without parameter selection. The selected calculation parameters are integrated into the method.

4. When indicated, use the **Save Method** command to store the method with the modified parameter selection.

   Tip: *Make sure that only those parameters are selected that are compatible with the wavelength range and the ordinate mode of the scan. Otherwise the result output will be canceled with an error message, resp.skipped.*

   Tip: *If no calculation is required, select the option* ***Insert Blank Line****.*

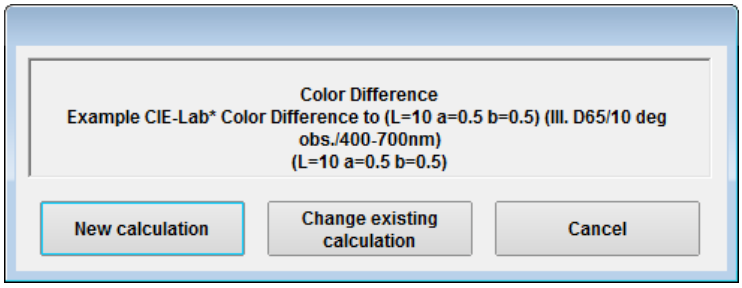
   The list of parameters, their designations and output options correspond to the entries in the **VL_ColorCalc.dta** parameter definition file. You can edit this file to modify the ordering, the parameter designations or output options. See: *Adapting the Evaluation Parameters* 8-17

Thickness Correction Option

The **Thickness correction** option allows you to recalculate a sample spectrum to a different sample thickness (path length). The **Thickness correction** status description **active** (in red) or **not active** shows the current setting of the path length correction option. Define the sample thickness transformation by clicking on the thickness correction **Setup** button. This opens the **Thickness correction** window. See: *Thickness Correction Window* 5-24.

Color Difference Setup

The color difference **Setup** button opens a dialog to modify an existing or to add an additional color difference calculation; see section *Color Difference* 7-8. The button is active, if at least one color difference calculation has been checked. If several color difference calculations have been checked, the function allows to select the definition to be edited. Further dialogs are presented in English; they do not use the local language of the installation.



Color difference definition

According to the required reference data, the dialog requests the required values, resp. uses the spectrum shown in the graph.

Important:

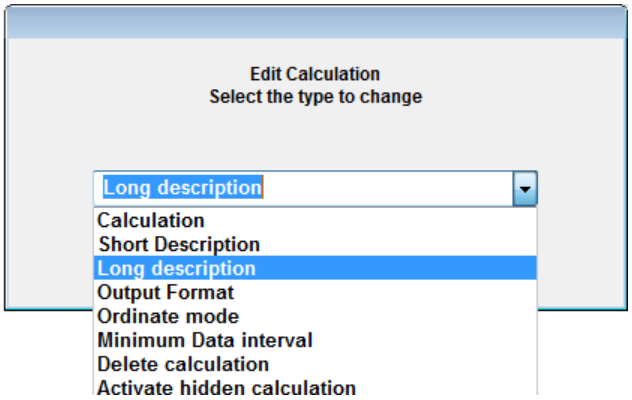
If a stored spectrum is used as a reference, this spectrum must be loaded to the graph beforehand. If no spectrum is present, the message "No spectrum available" is issued. If more than one spectrum is shown, the first spectrum is applied. The spectrum can be resident in the Results or in the superior Data directory.

Note: *If the text segment "Example" is found within the definition, as with the predefined color difference calculations, it is removed for the new definition.*

With each processing of the parameter definition file, an incremented backup file *VL_ColorCalc_*.dta* (starting at * = 001) is generated. The incrementation again begins with 001 after a new start of the software. Older backup file are overwritten without query.

Editing Parameter Definitions

The **Edit Calculation** button is available, if calculation definitions of the E- and M-type are selected in the method; see section *Syntax of Parameter Definitions* 8-18. The option allows modifying the calculation procedure and adding new calculations based on the selected one. Further dialogs are presented in English; they do not use the local language of the installation.



Edit Calculation selection

Additionally, the button is available for all types of calculation definitions, if the appropriate start switch is activated; see section *Options in the Software Start Line* 8-7. Then, the option additionally allows modifying the output format, the designations and other elements of the parameter definition. It also allows deleting parameter definitions and activating hidden parameter definitions. This option is recommended only for experienced users.

When clicking the **Edit Calculation** button and if more than one calculation definition is selected, the software queries, which of these is to be edited. Thereafter or if only one calculation definition is selected, the available editing options are presented in a dialogue. The dialog is only available in English. Make sure to strictly observe the syntax of the parameter definitions. See *Adapting the Evaluation Parameters* 8-17.

Note: *If the text segment "Example" is found within the definition, as with the predefined calculations, it is removed for the new definition.*

With each processing of the parameter definition file, an incremented backup file *VL_ColorCalc_*.dta* (starting at * = 001) is generated. The incrementation again begins with 001 after a new start of the software. Older backup file then are overwritten without query.

5.7.5 Thickness Correction Window

Define the sample thickness transformation by clicking on the **Thickness correction Setup** button in the **Calculations** window. This opens the **Thickness correction** window. The **Thickness Correction** option allows you to automatically recalculate a sample spectrum to a different sample thickness (path length). The applied procedure is applicable for transmission measurements on homogenous samples. See the section *Thickness correction* 7-3.

Define the sample thickness transformation in the **Thickness correction** window with the following steps:

1. In the main window click on the **Calculations** button.

2. In the **Calculations** window click the **Setup** button to open the **Thickness correction** window.

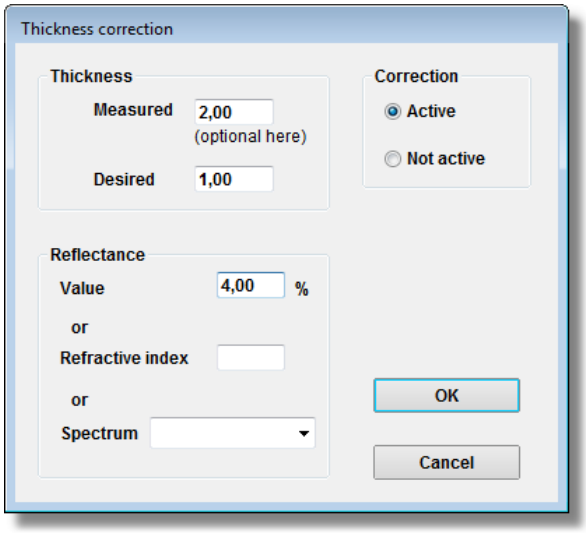


Figure: Thickness Correction window

3. In the **Correction** field select the option **active**.

4. Enter the current **Measured** sample thickness and the **desired** new thickness. Optionally you can omit the measured (actual) sample thickness entry: Then you must enter the thickness at each sample measurement in the **Sample information** window.

5. In the **Reflectance** group, enter either the reflectance **Value** for a single surface reflection or the sample's **Refractive index** value or the sample's single surface reflectance **Spectrum**. The default is a 4% reflectance value for a standard glass.

   Tip: *For thickness correction of liquid samples measured in cells, the reflection value is set to zero. Tus, the thickness correction just applies a simple ration calculation.*

6. Press **OK** to close the window.

   The thickness correction procedure generates an additional thickness corrected spectrum with the filename extended by **~corrected**. This spectrum is displayed in the graph, but it is not stored to disk automatically.
   The thickness correction entries are part of the method.

   Tip: *A thickness correction is not feasible for reflectance spectra scanned as **%R**. A warning is given if a method is to be saved with these options combined.*

   Tip: *If the thickness correction calculation generates net transmission values larger 100 %T within the spectrum, ambiguous measurements or wrong correction entries are probable. In this case a warning is added to the sample description of the thickness corrected spectrum.*

   See for more details of the applied principles the section *Thickness correction* 7-3

5.8 Graph Area

The graph area is the upper display section of the main program window. The graph area is activated if a spectrum is scanned or if a spectrum is loaded from disk via the command **Load Spectrum**. See: *File menu* 5-3

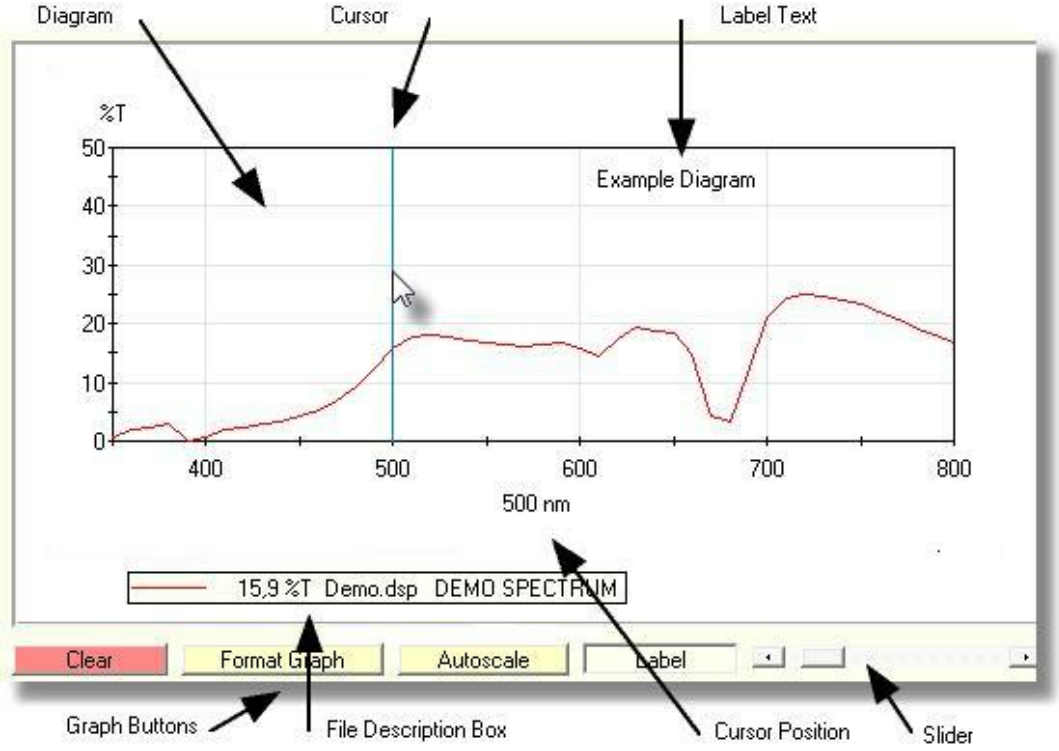


Figure: Graph area in the main window

The graph area consists of:

- The graph with the file description box and optional automatic cursor.
- The graph buttons providing access to several graph tools.

By modifying the program window size you can modify the graph area size. The split between the graph area and the results area can be varied at the upper margin of the results area: Position the mouse pointer at the separating line and drag the margin while pressing the left mouse key.

Graph

The graph is annotated on the x-axis (abscissa) with wavelength (nm) and on the y-axis (ordinate) with the ordinate type of the spectrum/spectra.

Colors are used for overlaid curves in a fixed order. Up to 20 curves can be displayed. This number can be configured to up to 50. See: *Software Configuration* 8-3. If more spectra are loaded or measured, the oldest spectrum is exchanged at the time.

For measured data, the graph's scaling corresponds to the method settings. When spectra are loaded from disk, the scaling is adapted automatically (Autoscale). The scaling can be changed via the graph tools (see below) or via the expansion functions. Use the **Autoscale** button or

double-click the graph will return to the autoscale presentation.

When spectra with different ordinate modes are displayed, the left y-axis is used for the first ordinate and the right axes is used for the second ordinate.

Note: *There must be at least on spectrum correlated to the left y-axis. When the last spectrum of the left Y-axis is deleted, also all spectra correlated to the right axes are deleted.*

Expansion of Details

You can expand deliberately a rectangular area or an abscissa range of the graph.

Expanding an Area of the Graph

1. Position the mouse pointer at any corner point of the rectangular area to be expanded.
2. Then drag the mouse pointer with pressed left mouse button over the area to be expanded. The area will be framed.
3. After releasing the mouse button the framed area is expanded to the full size of the graph.

Expanding a Selected Abscissa Section

1. Position the mouse pointer at the left or right edge of the area to be expanded.
2. Then hold the [Shift] key and drag the mouse pointer with pressed left mouse button over the area to be expanded. The area will be shown in inverse colors.
3. After releasing the mouse button the highlighted area will be expanded to the full size of the graph with unmodified ordinate scaling. A slider is additionally available; see below.

The expansion slider becomes active after expansion. To return to the default expansion use the **Autoscale** button. See below: *Graph Tools*

Graph Buttons

The following operational elements are available for the graph:

Table: Tools used with the graph

Tool	Function
Clear button	The red **Clear** button deletes ALL curves in the graph. If you want to delete only single curves, use the specific **File Information** Window.
Format Graph button	This button opens a window with a schematic coordinate system. You can enter the desired ordinate and abscissa minimum and maximum values. You can step from one field to the next using the tab key.
Autoscale button	The **Autoscale** button resets the scaling to default values, which are abscissa and ordinate ranges that fully display all the curves. The ordinate range is automatically selected so that all data points are displayed. During scanning the **Autoscale** button only operates in the y-direction to show the continuation of the curve. ***Tip:*** *Double-clicking the graph executes the same function.* ***Tip:*** *Entering **0.0** for both **Y-axis minimum** and **Y-axis maximum** generates*

Tool	Function
	an "autoscale" during measurements.
Label text entry field	Click on the text entry field and move it with pressed left mouse key to any desired position within the graph. After release of the mouse key, a text entry field opens. Enter the required label text. The text may use several lines. This text is displayed at the label position.The position of the text is assigned to the graph scaling. Therefore, the text will change its position, when changing the scaling of the graph. ***Note:*** *When all spectra in the graph area are deleted, also the label texts are removed.*
Expansion slider	The slider is only active if the spectrum/spectra are not displayed with their full abscissa range. The slider allows you to move the expanded section and depicts the position of the section in respect to the full abscissa range.

Tip: *The graph buttons normally are inactive during measurement except for the* ***Autoscale*** *button.*
The configuration option "GraphAccessScan" in the configuration file allows defining that the other graph buttons are accessible and that additional spectra can be loaded. See Configuration File 8-3.
Then, in case that an operation takes too much time, e.g. when a menu stays open by accident, the spectrometer will stop scanning after a certain time. This situation should be avoided, because the spectrometer might not continue properly.

Cursor

Whenever you move the mouse pointer into the graph, a blue cursor line is added to the graph that follows the mouse movement. The normal vertical cursor (also just "cursor") and a horizontal cursor is available.

The vertical cursor is shown, when the mouse pointer is moved into the graph area through the X-axis or from the top. The horizontal cursor appears, if the mouse pointer enters the graph through the Y-axis (from left or right). See below *Using the horizontal cursor.* The cursors automatically disappear, when the mouse pointer is moved out of the graph.

When a cursor is active, the current cursor abscissa position is displayed below the abscissa axis.

Also with the vertical cursor, the corresponding ordinate value of the curve(s) is shown in the **File description** box. Values are taken from the nearest measured data point. See below the sections *File Description Box.*

The vertical cursor is employed to transfer ordinate/abscissa values of the curve(s) to the results area. See below *Read Cursor Mode*.

Using the Horizontal Cursor

The horizontal cursor appears automatically, when the mouse pointer is introduced to the graph from the left ordinate.

The horizontal cursor allows a quick check of the abscissa position(s) for certain ordinate values of the curve(s): When the horizontal cursor is active, the **File description** box shows the abscissa value (wavelength/time) of the intersection point with the curve to the right. The horizontal cursors in the vertical steps with the digits of the third significant position (e.g. 25.1 - 25.2 - 25.3). The *GraphYCursorRounding* parameter of the configuration file allows changing to the fourth significant position.

If there are several intersection points for a curve, the next intersection point to the right is shown. Other intersection points are shown by moving the cursor accordingly.

Read Cursor Mode

The **Read Cursor** mode allows transferring spectral data at the cursor position to the results space.

- In the **Spectrum** information windows of the spectrum to be evaluated, the **Read Cursor** button activates the mode. See: *Spectrum Information Window* 5-30. You may use the **apply to all** option to simultaneously read all spectra in the graph.
- In response, the **Spectrum** information window is closed and the cursor is placed in the graph area. The mouse pointer changes to a cross.
- Pressing the left mouse key will insert a table in the result area. Ordinate and abscissa of the spectra/spectrum at the current cursor position(s) are entered into that table with each mouse click. See: *Results Area* 5-32

Note: *Make sure that the mouse is not moved while pressing the left mouse key, because this will be interpreted as scale expansion.*

To close the **Read Cursor** mode just move the cursor out of the graph area.

Note: *Cursor data are added to existing results. Any new spectrum evaluation however will delete the* ***Read Cursor*** *table.*

File Description Box

The file description box lists all curves currently displayed in the graph with:

- Color of the curve
- Current cursor ordinate value (if the cursor is active, see above)
- Filename
- Sample description

See also: *Sample Information Window* 6-2

Note: *The additional sample information is shown with its designation, if the parameter SpectrumLong in the configuration file is set. If however, the complete text has more than 80 characters, the designations are left out.*

The spectra are listed in the order of their measurement or loading.

If the mouse pointer is moved into the file description box it changes into a hand symbol. This is to draw your attention to the option to click on a filename. This will open the *Spectrum information window* 5-30.

Note: *This option is not available, if another function is active e.g. another window or a menu.*

Graph-Layout Configuration

This option is only available with the additionally installed **Reporter-SPX** software. When right-clicking on the graph area, the **Chart Control** properties window opens that allows configuring the graph layout. See: *Report Configuration* 8-35 and the *Reporter-SPX Operator's Manual.*

5.8.1 Spectrum Information Window

When you move the mouse over a spectrum filename in the file description box, the mouse pointer changes to a hand. Clicking the entry, opens the **Spectrum** information window for the spectrum. The window shows the spectrum filename in its header and it lists the parameters of the selected spectrum:

- Sample description (as entered with the sample information window), see *Sample information window* 6-2.
  Alternatively, the additional sample information is shown with its descriptions. See *Advanced Options window* 5-21.

- Operator (as entered with the sample information window), see *Sample information window* 6-2.

- Date of measurement and date of last modification (modifications can be, for example, **A<>% T** transformations or editing the sample description. If no date of modification is given, the file has not yet been modified.)

- Abscissa and ordinate ranges, data interval, number of data points, and the measurement wavelength (for loaded rate data sets)

- Type of spectrophotometer with serial number and firmware revision, if available. See: *Spectrometer and Accessories* 10-1

- Spectrophotometer settings, e.g. integration time and applied accessory

- Date the associated baseline correction has been performed

- Software version

- Audit trail – this is information about generation of and manipulations to the spectrum, i.e. reflectance correction or renaming.

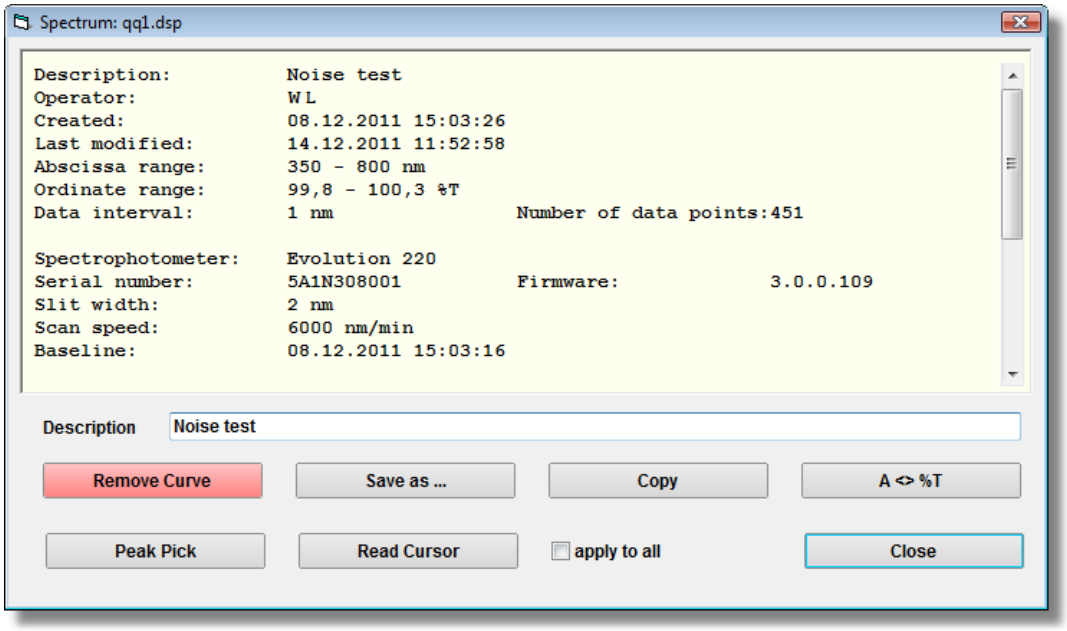


Figure: Spectrum Information window

The entry box **Description** allows modifying the spectrum description.

In addition, the **Spectrum** information window offers buttons for the functions listed in the following table.

*Table: Functions offered in the **Spectrum** information window*

Button	Function
Remove Curve	Deletes the selected curve from the list of displayed files. If you selected the **apply to all** option, all spectra in the graph will be removed.
Peak Pick	Starts a peak pick routine for the selected data file. Parameters for peak picking (**Maxima, Minima** and **Maxima**/**Minima** as well as (peak-)**Threshold**) are queried in further dialog windows. The detected extrema are numbered in the graph and they are listed in the results area. See *Results Area* 5-32. If you select the **apply to all** option, all spectra in the graph will be considered.
Read Cursor	Starts the **Read Cursor** mode. This mode allows transferring spectral data at the cursor position to the results space, see *Read Cursor mode* 5-29. If you selected the **apply to all** option, all spectra in the graph will be considered.
Save as	Opens a **File Save as** window to save the spectrum/spectra as an ***.dsp**, ***.csv** or ***.dx** file. (See: *Data Formats and Spectrum Import/Export* 9-1). The results directory defined in the **Preferences** command is used as the default directory. See: *Preferences* 5-12 If you selected the **apply to all** option, all spectra subsequently will be offered for storage. ***Tip:** Each recorded spectrum is stored after measurement. This function allows storing spectra under a different name, at a different directory or in a different format.*
Copy	Copies the spectrum/spectra to the clipboard as a table. These data can be

Button	Function
	pasted for example to a spreadsheet software. If you selected the **apply to all** option, a table containing the data of all spectra in the graph will be generated. ***Tip:*** *Copying more than 1 file to the clipboard is only recommended, when the spectra have the same wavelength range and data interval. If not, copy the spectra separately.*
A<>%T	Transforms the selected data file from **A** to **%T** and vice versa. **%R** spectra are transformed to the **Log 1/R** ordinate mode. Spectra with **%Ra** and **f(R)** are not transformed. If you selected the **apply to all** option, all spectra in the graph will be transformed.
Close	Closes the **Spectrum** information window.

5.9 Results Area

The results area is in the lower right section of the main window (See: *Software Operation)* 5-1 and is used to present the alphanumerical results calculated for the spectra displayed in the graph area, and the cursor readings. Results are listed separately for each spectrum together with its name and description.

In order to evaluate several spectra simultaneously, it is necessary that the spectra are present in the graph. For spectra measured on-line, this means that the option **Graph Overlay** / **Permanent** must be active.

Tip: *When calculations in reference to another spectrum are selected as calculation parameters (e.g. color difference), the reference spectrum is not evaluated.*

When results has been generated, the following options are available:

- The split of the graph and the results areas can be varied at the upper margin of the results area: Place the mouse pointer on the edge and drag the margin while pressing the left mouse key.
- Use the window slider to show hidden results.
- Use the **Export results** command to generate a result file in csv-format. See *File Menu* 5-3.
- Print the results together with the graph via the **Print** command or the **Print** button. The **Print Preview** command opens the **Print Preview** windows for the report printout. See: *Print commands* 5-5 and *Print Preview* 5-6

Tip: *By installing an additional template (See: Templates for Data Handling* 8-12*) the* ***CommentResults*** *function can be implemented. This allows adding additional information to the results area.*

Tip: *With the additionally installed* ***Reporter-SPX*** *software the* ***Export*** *function in the* ***File*** *menu is available to save the report with a choice of formats.*

Transfer Results to the Clipboard

You can copy the presented results partially or completely to the clipboard for further use in other softwares:

1. Click on the result area.

2. If you only want to transfer the result partially, mark the required section (by pressed left mouse key).

3. Use the [Ctrl] + [C] key combination to transfer the text of the results area to the clipboard.
   If you mark the text partially (with pressed left mouse button) only the marked text is transferred.

4. From the clipboard, you can paste the information into other software with the software's **Paste** command.

Tip: *Via the **Print Preview** you can copy the full report including graphics to the clipboard. See: Print Preview* 5-6

Tip: *The report can also be copied to clipboard in a tabular format with the additional Copy Result table to Clipboard template. See: Templates for Data Handling* 8-12.

5.10 Recalculation

The **Recalculate** button in the operating toolbar is used to perform a new calculation of results for the spectra displayed in the graph area. (See: *Operating Toolbar* 5-2 and *Graph Area* 5-26) The calculation parameters can be identical or can be modified by loading a different method or via the **Calculations** button in the parameter. See: *Calculations Window* 5-21.

As well, previously recorded spectra can be (additionally) loaded with the **Load Spectrum** command and can be re-evaluated. See: *File Menu* 5-3

Tip: *When several spectra are to be evaluated simultaneously, they must all be displayed in the graph area.*

Tip: *Automatic printout with the **Autoprint** option or automatic report storage with the **Autosave** option is not possible with the recalculation. Use the **Print** button for printing the report or the **-> PDF** button to save the report as a PDF file. You may also use the **Copy to Clipboard** command to transfer the report to the clipboard and paste it to another program for storage from there.*

Tip: *With the additionally installed **Reporter-SPX** software an **Export** command is added. This command allows storing reports in different formats. See: Results Area* 5-32 *and Report Configuration* 8-35

Note: *Spectra, which have been recorded with an individual, actual sample thickness have this information saved in the data file. For a recalculation of such spectra with the thickness correction activated, but no actual sample thickness given, the saved thickness value is applied. If the recalculation with a different actual sample thickness is required, this value must be entered in the method as the actual **measured** sample thickness in the **Thickness Correction** window.. See: Thickness Correction* 7-3

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6 Measurement

To perform a measurement, either select a method or modify the parameter settings of the current method, as required. See: *Parameter Area* 5-15 and *Overview* 4-1

Data recording, data evaluation, and result output settings are defined within methods. Thus, you can save and restore standard parameter settings for routine measurements. Method files are characterized by the file extension **mol**.

Note: *Make sure that the scan range covers at least all wavelengths necessary for the defined calculations. The data interval can be selected freely. However data intervals larger than 5 nm should not be selected in order to maintain a sufficient result accuracy. See: Calculations Window* 5-21

If you want to use the selected parameter settings for future measurements, save the settings as a method file via the **Save method** command. See: *Overview* 4-1

If a suitable baseline run under the selected conditions has not yet been performed, perform a baseline run in advance via the **Baseline** button. Alternatively you will be requested to perform a baseline run in the **Sample Information** Window.

Note: *If a baseline correction run is canceled, no baseline correction data are stored.*

With relevant modification of instrument settings like slit setting or the lamp change point, a new baseline run should be done too, even if the software does not request it expressively.

To Perform a Measurement

A typical measurement is executed with the following steps:

1. Select a method in the **Method** list box,
   or alternatively
   modify the measurements settings and/or open the **Calculations** window with the **Calculations** button and modify the calculation parameters. See: *Overview* 4-1 and *Calculations Window* 5-21

2. Optional: To measure the baseline in advance, click the **Baseline** button to start a baseline run with the selected settings using the appropriate blank or an empty sample position.

3. Click the **Measure Samples** button to start the measurement with the selected settings. The **Sample information** window is presented. See: *Sample Information Window* 6-2. If not done in step 2, insert the blank into the sample compartment and close the sample compartment cover. Hit the return key or click **OK** or (for sipper operation) click the **Measure** or **Measure and Sip** button or press the sipper key (at the sipper) to start data recording. The baseline correction data will be recorded and displayed.

4. After termination, the **Sample information** window is opened again. Enter the information for the next sample or define the sample information for a batch of samples. See *Sample List Operation* 6-5.

5. Hit the return key or click **OK** or (for sipper operation) click the **Measure** or **Measure and Sip** button or press the sipper key (at the sipper) to start data recording. The sample spectrum will be recorded and displayed according to the selected settings.
   With the entry **0.0** for both **Y-axis minimum** and **Y-axis maximum** the graph is continuously adapted to the data during measurement.

6. If you want to cancel a measurement during progress, use the **Stop** button in the toolbar. See: *Operating Toolbar* 5-2

7. After a measurement, the resulting spectrum is displayed in the graph and the results are listed, see *Results area* 5-32.

8. A new **Sample Information** window is displayed for the next sample. Continue as above or use the **Close** button to terminate the series of measurements.

   Click the **File/Print Preview** function to view the report or click the **Print** button to print it. The report contains all required evaluation results together with the spectrum graph. See: *Print Commands* 5-5

   Tip: *Stored spectra can be loaded and can be re-evaluated via the* ***Recalculate*** *button. See: Operating Toolbar* 5-2 *and Recalculation* 5-33

6.1 Sample Information Window

In the **Sample Information** window, you define the next sample or the sample group in cell changer mode to be measured. Alternatively you can define a sample list (not in cell changer mode). See: *Sample List* 6-5.
You can define a baseline run at any time by activating the **Measure blank** checkbox.

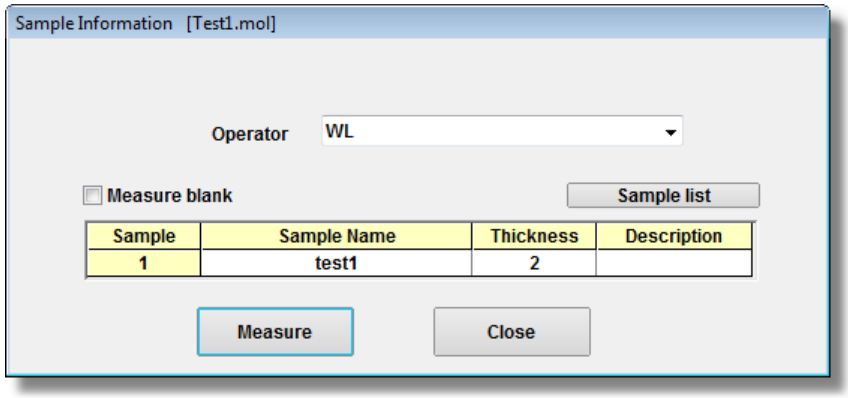

Figure: Sample information window (Thickness column only with Thickness correction activated)

The following entries are possible:

Operator

The **Sample information** window allows entering an **Operator** name. If available, the name of the current Windows user is entered as a default. The user name will also be stored in the spectrum information.
The dropdown arrow besides the entry box allows selecting previous entries, see below.

Sample Name

The **Sample Name** is mandatory for the measurement. The **Sample Name** is used as the filename for the automatic storage of the spectrum. Therefore the entry must follow the guidelines for Windows filenames.

If the last character is a digit, the sample name will be automatically incremented within a series of measurements.

Note: *The filename may have up to 251 characters including the path designation. The following characters are not allowed:*

\ / : * ? " < > |

The filename should not be too long, since the presentation partially is truncated and since some other programs do not cope with very long filenames.

Important:

If you select a filename that already exists, you are asked if the existing file can be overwritten. If this has been accepted, ***another entry of the same filename will not again be prompted for overwriting.***

Thickness

The sample **Thickness** entry field is displayed, if the thickness correction option has been set to **Active** and the sample thickness value was not entered in the **Thickness Correction** setup. This entry is mandatory, since the figure is required for the calculations. See: *Thickness Correction* 7-3.

Additional, user-defined sample information

Up to 6 additional sample information items that are user-defined in the method. See *Advanced Options Window* 5-21.
The width of the columns is equivalent to the length of the defined **Designation**. Overall, up to 110 characters can be shown.

Description

Optional, informative text. Not shown, if an additional **Sample Information** is defined (see above). The **Description** entry is stored with the data file and is used to document sample details. There is no restriction on the length of the entries. The entry can be checked in graph legend and can be modified in the **Spectrum** information window. See: *Spectrum information Window* 5-30.

Tip: *The description entry field is cleared for each new sample within a series of samples. If you should wish to keep the description entry for successive samples, this can be configured. See: Options in the Configuration File* 8-3.

When a list of samples to be measured is available, the samples data can be collectively entered before the measurements are started. Click on the **Sample List** button (only available with the first sample of a measurement series) to extend the sample table to 1000 lines. See: *Sample List* 6-5

Alternatively you can open the context menu by clicking the right mouse button. A sample list can be loaded. Other functions are as described in the sample list section. See: *Sample List* 6-5.

Operator

The window has an **Operator** text box. The entry is initially taken from the Windows user administration. As a default, it has the format:

Domain or PC-name \ login name (full user name)

Other compositions can be configured. See: *Defining the User Name Appearance* 8-2.

The entry can be overwritten by a user entry. This will be applied as the new default for the following measurements.

To facilitate an entry with various operators, a list of up to 25 **Operator** names is maintained that use the software under the same Windows login. With the drop down arrow at the end of the entry box, an entry can be selected from that list. The list is held in the user-specific configuration file. See: *User configuration file* 8-2.

Sample Information

Sample name and sample characteristics (**Description, Dilution Factor** and additional sample information) are entered within the sample line or table. The table column width can be varied by dragging the separating line of the header line to the desired position.

Note: *The **Sample Names** are used as Windows filenames. Thus, Windows conventions must be followed: maximum length of 215 characters (including spaces). You may not use the following characters: \ / : * ? " < > |.*
Generally, avoid using extensively long filenames: When space is insufficient in an output, entries will be truncated in the middle or at the end.

The automatic incrementing of sample names can be disabled in the configuration file. See: *Software Configurations* 8-3.

In the configuration file you can preselect to take the description and dilution factor of the most recently performed measurement series. See: *Software Configurations* 8-3.

Tip: *Clicking the sample information with the right-mouse key opens a popup menu. The functions of this menu allow handling the entries. For example use the **Paste** function to insert clipboard contents or select **Delete** to remove an entry. See also: Using a Sample List* 6-5.

If an existing filename is entered, a query is issued to overwrite the existing results.

Important:
If you accept overwriting at this point and enter the same filename for another measurement series again, it is assumed that the existing file should again be overwritten: no further overwrite query will be shown.

Other Details

Other details presented in the **Sample information** window depend on the associated accessory:

- In the cell changer mode the **Sample Information** window displays as many lines as the cell changer provides cell locations. Only those locations are measured that have consecutive sample name entries. Functions for editing the list are equivalent to those described for the sample list.

Note: *With a cell changer the autozero/background measurement is always done on cell changer position 1.*

- In sipper mode the **Sample Information** window additionally presents buttons to operate the sipper. You start data recording by clicking the **Measure** or **Measure and Sip** button, or press the sipper key (at the sipper). The sipper settings are defined using the **Accessory** button (only available if applicable) in the **Spectrophotometer** area. See: *Spectrometer and Accessories* 10-1 and *Options in the Configuration File* 8-3

Baseline/Autozero in the sample information window

If no baseline run has been performed for the required wavelength range, you will be requested in

the **Sample information** window to do this. In the first line of the sample table, the **Sample name** field is designated as **Blank**. You cannot modify this entry (as shown by the blue field). Alternatively, you may use the **Baseline** button of the tool bar beforehand.

Where applicable, insert the blank cell/sample instrument or clear the sample position and start the run.

Tip: *For service purposes, the enforced baseline correction can be switched on/off by setting of the configuration file. See: Options in the Configuration File* 8-3

If a baseline/autozero run has already been performed, it is still possible to repeat this – and also at any time within a series of samples – by checking the **Measure Blank** selection box above the table. If this option has been used, it will be the default setting for the following measurements. In cell changer mode, the first position will then be reserved for the blank accordingly. To reset this behaviour, deselect the **Measure Blank** option anytime.

6.2 Sample List

Normally, the software prompts the user for each new sample. Via the context menu of the sample information entry, via the **Sample list** function or with the cell changer mode, you can enter or import sample information for a batch of samples in advance. This is especially relevant for serial measurements with a sipper.

After starting a method, the **Sample information** window offers the button **Sample list** *with the first sample*. Click on this button to extend the sample data area to 1000 lines. See: *Sample Information Window* 6-2

Note: *In cell changer mode the sample table has a number of lines equivalent to the number of cell changer positions. The **Sample list** button is not offered.*

Sample information entry to the table is done similar to a spreadsheet program. Sample data are entered line by line ***without empty lines***. An error message is issued, when inconsistent entries are detected. Sample names must be unique as the sample names are used as filenames for the automatic spectrum storage.

Tip: *Large sample lists should be prepared by external software as described below, (see: Storing and Importing a Sample List) since the software offers only limited editing functions.*

Editing a Sample List

When the table is opened, the first cell is marked (shaded frame). New information can be entered. Double click the cell to edit information. Accordingly, the cell shows a blinking vertical entry cursor (edit mode).

- Right-clicking a cell in the edit mode opens a standard edit context menu, which allows reversing the action, copying/pasting texts and more.
- Right-clicking a marked cell opens the table context menu with the functions described in the table below.

Use the cursor keys (in edit mode not right/left) or the Tab key on the keyboard or click a cell with the mouse to change to the desired cell. Then the cell is marked.

Table: Commands in the table context menu

Command	Function
Delete	Deletes the entries of the marked cell or of the cell area marked previously.
Delete line, Insert line	Adds or deletes a single line at the marked position. ***Tip:*** *You can also use the [Del], [End], [Ctrl+C] and [Ctrl+V] keys.*
Open file	Re-loads an already stored sample list (see below)
Save as	Stores the currently displayed sample list (see below)
Copy from clipboard	Pastes a properly formatted sample list via clipboard (see below). Using this function allows you to put together a sample list from different sources.

Tip: *The commands refer to the currently marked cell(s). To mark an area, move the mouse over the required area with the left mouse key pressed.*

Fill down Function

With a multi-line sample information table (cell changer or sample list) you can use the **Fill down** button to transfer the contents of the active cell to all cells beneath. Sample names are automatically incremented, when the last character is a figure.

1. Click on the cell to be transferred.
2. Click the **Fill down** button, to transfer the content of the marked cell to all cells below.

   Alternatively mark the required cell entry and an area below. The **Fill down** function then will only fill the marked area with the contents of the uppermost cell of the selected area.

Tip: *You use the **Delete** function of the table's context menu to remove an entry. To delete several redundant entries, it is possible to use the **Fill down** function to transfer an empty cell.*

Storing a Sample List

Sample lists can be handled as a file for repeated use. Sample list files are text files, which can be generated externally or by the software in the **Sample information** window. Sample list files use the file extension **.lol**. They are stored in the current method directory.

When editing a sample list table, the table context menu offers the command **Save as** to store the sample list; see above. The file format is:

sample/spectrum file name1(<Tab>sample1 thickness, if applicable)<Tab>spectrum description1
sample/spectrum file name2(<Tab>sample2 thickness, if applicable)<Tab>spectrum description2
etc. (with 2 advance empty header lines)

Tip: *When selecting the name of the current method as the sample list name, this sample list will be linked to the method: The sample list will then be loaded automatically with the next use of the method.*

Sample list files can also be generated by an external text software like the Windows Notepad/ Editor following the above format. The empty header lines may be omitted. Instead of the <Tab> character also the Windows line separator character can be applied. When storing the sample list file, make sure to use the proper method directory path and the proper file extension.

Tip: *It is possible to generate a sample list leaving the filename information empty. This would allow to just give some information for the samples to be measured in the* ***Description*** *section.*

Loading/Importing a Sample List

The **Open file** command of the sample list context menu loads the sample list for the following measurement. The software will enter the sample information beginning with the first line.

When selecting the name of the current method as the sample list name, this sample list will be linked to the method: The sample list will then be loaded automatically with the next use of the method.
Tipp: *If the second header line of the sample list (the firs header line is empty) then contains the code ";;MO_MEASURE", a measurement is started immediately.*

Tipp: The *AutoIncrement* option of the configuration file allows using incremented spectrum file names without changing the sample list. See: *Options in the Configuration File* 8-3. When a sample list holds sample names ending with digits, the system will check the results directory for the presence of spectrum files with the same root filename ending with digits. If such files exist in the results directory, the filename digits are automatically adjusted to avoid accidental file overwriting.

Alternatively to loading a sample list file it is also possible to paste sample information via clipboard. Use the **Copy from clipboard** command in the table context menu, if a properly formatted sample list has been copied to the clipboard. The information will be pasted beginning with the active cell. Thus it becomes possible to put together a sample list from different sources.

6.3 Data Recording

If the **Sample Information** window is shown, start the measurement by clicking on the **Measure** button or by pressing the ENTER key of the keyboard.

When the external Peltier temperature control is active, the measurement may be halted, until the required temperature has been reached. A message window is shown.

If a wait time has been defined, the defined time is counted down in a dedicated window. See *Advanced Options Window* 5-21.

During the run, the flashing **Stop** button of the operating tool bar is presented so that you can cancel the run at any time. See: *Operating Toolbar* 5-2. the data are shown in the graph area and in the live display, if technically possible with the specific instrument. See: *Spectrometer and Accessories* 10-1.
The graph buttons normally are inactive during measurement except for the **Autoscale** button.

Tip: *The configuration option "GraphAccessScan" in the configuration file allows defining that the other graph buttons are accessible and that additional spectra can be loaded. See Configuration file* 8-3.

The recorded spectra are automatically saved to disk in the results directory with the selected

sample name as the filename and the extension **.dsp**. See: *Preferences* 5-12, and *Sample Information Window* 6-2

After the run, the alphanumerical results are presented in the results area and the report is printed and/or saved automatically, if defined in the method. If the report uses a method specific page layout (e.g. with the additionally installed **Reporter-SPX** software), the new report is shown in the **Print Preview** window. See: *Print Preview* 5-6

Note: *If the calculation of a parameter is not possible, an error message will be issued and the report generation will be canceled. With the wrong ordinate mode, the calculation is skipped. Thus the report may be incomplete.*

When **Repetitive measurements** have been defined for this measurement, the next scan will be initiated automatically after the selected interval time. See *Advanced Options Window* 5-21.

The next sample information window is presented. If a sample list is used, the data of the next predefined sample are displayed.

6.4 End of Measurement

After the measurement of the current sample or sample group, the **Sample information** window for the next sample/sample group is presented (not when using a sample list). Proceed with the next measurement, or stop the measurement series with the **Close** button.

Thereafter you can start another series of measurements or perform the following tasks:

- Print the report via the **Print** button.
- Open the **Print preview** window e.g. to store the report as a PDF file.
- **Export** the result values as a csv file.
- Use the **Recalculate** button to re-run the calculations with modified parameters. See: *Recalculation* 5-33
- Use the various features of the graphics window (e.g. to export spectra). See: *Graph Area* 5-26

If you plan another measurement with similar sample(s) you again start the measurement via the **Measure Samples** button. If you plan another measurement with a new method, select the new method or modify the parameter settings accordingly. See: *Operating Toolbar* 5-2

6.5 Results Storage

The recorded spectra and the results are stored independently.

Sample Spectra

The recorded sample spectra principally are stored in the results directory with the selected name. Thus they are available for a re-calculation. The standard format is a proprietary format with the extension **.dsp**. See: *Data Formats* 9-1

The configuration file (parameter **sp_ext**) alternatively can define that the spectra generally are stored in the JCAMP-DX format or in the **.csv** format. The selected format can be assigned with another file extension (**ExportExt**, **JCAMPExt**) and with specific settings (**ExportFormat**, **JCAMPFormat**). See: *Software Configuration* 8-1.

Spectra residing in the graph additionally can be stored with another name and/or to another directory (**File/Save Spectrum as** or in the **Spectrum** information window.)

Copying a single or several spectra to the clipboard in a tabular form is made possible in the **Spectrum** information window. See: *Spectrum information window* 5-30.

Results

The report is automatically stored to the results directory as a PDF file after data recording, if the **Save automatically** option is active. The report includes spectrum graphics and calculation results.

The filename for this and the other report storage options is that of the spectrum or the first spectrum of a series. Further storage options are:

- If the configuration file defines an export directory for text results (**TextResultsPath**), results are additionally stored in this directory as a text file for further use. The file extension can be defined (parameter **TextExt**). This is independent of the **Save automatically** option.

- As well, the configuration file can define an export directory for an additional PDF result storage (parameter **PDFResultsPath**). This is independent of the **Save automatically** option.

- If the configuration file defines an export directory for results (**ExportResultsPath**), results are additionally stored in tabular form as a **csv**-file in the given directory. This is independent of the **Save automatically** option.

Furthermore, the complete report can be copy/pasted from the **Print Preview** window and the results can be copy/pasted from the results space. See: *Print Preview* 5-6 and *Results Area.* 5-32

When the additional **Reporter-SPX** software is installed, the **Export** function is available to store the results in a number of further formats.

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7 Evaluation Parameters

The software offers the calculation of a wide choice of parameters from the recorded sample spectrum. See the list of available parameters below. Further details about selected parameters are given in this section. You can find further information about the parameters in the respective standards and norms.

The following list of the calculation parameters is based on the parameter definition text file **VL_ColorCalc.dta** in the Data directory. Editing this file allows removing unwanted parameters, changing the order and the output texts or adapting the enclosed examples. See: *Adapting the Evaluation Parameters* 8-17

Note: *With spectrometer models with limited wavelength range or if a required accessory (esp. integrating sphere) is not applicable, some of the parameters offered by the software cannot be executed.*

Table: Evaluated parameters and required wavelength range

Color Values (reduced wavelength range) (2)	
XYZ tristimulus color values (A,C,D65; 2,10 deg)	400-700 nm
xyY color coordinates (A,C,D65; 2,10 deg)	"
CIE L*a*b* color values (A,C,D65; 2,10 deg)	"
CIE L*C*h* color values (A,C,D65; 2,10 deg)	"
Color Values (extended wavelength range) (2)	
XYZ tristimulus color values (A,C,D65; 2,10 deg)	380-780 nm
xyY color coordinates (A,C,D65; 2,10 deg)	"
CIE L*a*b* color values (A,C,D65; 2,10 deg)	"
CIE L*C*h* color values (A,C,D65; 2,10 deg)	"
Color Values (full wavelength range) (2)	
XYZ tristimulus color values (A, D65; 2,10 deg)	360-830 nm
xyY color coordinates (A, D65; 2,10 deg)	"
CIE L*a*b* color values (A, D65; 2,10 deg)	"
CIE L*C*h* color values (A, D65; 2,10 deg)	"
CIE L*a*b* Color Values with further illuminants (extended wavelength range/ 5 nm) (2)	
CIE L*a*b* color values (F2, F7, F11, D50, D55, D75; 2,10 deg)	380-780 nm
Dominant Wavelength, etc. (2)	"
Dominant wavelength, Complementary wavelength, Excitation purity, Colorimetric purity	380-780 nm

(1) With these parameters the ordinate mode is disregarded. When spectra are required in %T or %R, spectra supplied in absorbance (A) may give erroneous results.
(2) With these parameters, spectra in absorbance (A) are transformed to %T before calculation.
(3) This parameter is only executed for reflectance spectra.

Examples: Color Difference (2)	
CIE color difference values to L*a*b* reference values (A, C, D65; 2,10 deg), example	380-780 nm
CIE color difference values to X, Y, Z reference values (A, C, D65; 2,10 deg), example	"
CIE color difference values to reference spectrum (A, C, D65; 2,10 deg), example	"
CMC (2:1);(1:1) color difference values to L*a*b* reference values (D65/10), example	"
CMC (2:1);(1:1) color difference values to reference spectrum (D65/10), example	"
DECIE2000 (1:1:1) color difference values to L*a*b* reference values (D65/10), example	"
DECIE2000 (1:1:1) color difference values to reference spectrum (D65/10), example	"
Whiteness, Yellowness, Tint (2)	
Whiteness Index (CIE 1982), (Ganz), (ASTM E313-05)	380-780 nm
Yellowness Index (ASTM 1925), (ASTM E313-05)	"
Tint Values (ASTM E313-05)	"
Color Evaluation according to European Pharmacopoeia (2)	
Color comparison for B5-B9, BG4-BG7, G4-G7, GG4-GG7, R4-R7 (1 cm and 5 cm)	400-700 nm
Simple, Uni-dimensional Color Values (2)	
Pt-Co/Apha/Hazen Color Value (1, 5, 10 cm) (DIN 53409, ISO/DIS 6271)	380-780 nm
Gardner Color Value (1 cm) (ISO/DIS 4630-2)	"
Gardner Color Value, fractional part (1 cm) (ISO/DIS 4630-2)	"
Iodine Color Value (1 cm) (DIN 6162)	"
Saybolt (10 cm) and ASTM (33 mm) Color Value (ASTM D6045)	"
Calculations with uni-dimensional Color Values - Examples	
Pt-Co/APHA/Hazen-Color Value (1 cm), example	"
Gardner Color Value Comparison/Check, example	"
Iodine Color Value Comparison/Check, example	"
Color of Wines (1)	
Abs (420 nm), (520 nm), (620 nm)	420, 520, 620 nm
Diff. Abs (520 nm) to proceeding spectrum	520 nm
Peak Abs (Peak 510-540 nm)	510-540 nm
Net Peak Abs (haze corrected) (Peak 510-540 nm/700 nm)	510-700 nm
Tonality Sudraud (420/520 nm)	420-520 nm
Color Intensity Glories (420/520/620 nm)	420-620 nm

Color Intensity reduced (420/520 nm)	420-520 nm
Color Intensity (haze corrected) peak (420/Peak 510-540 nm/700 nm)	420-700 nm
Polymeric Color Ratio	420-700 nm
Color Percentages yellow, red, blue	420-620 nm
Mean Value and Coefficient of Variation Calculations (1/2)	
Averages and coefficient of variation for 2, 5 and 10 measurements for parameters 1 and 2	-
Examples : Numerical Calculations (1)	
Comparison to min/max spectra, example	400–600 nm
Comparison to min/max spectra, example	within 200-1100 nm
Calculations with spectral data, examples	various
Sample classification according to LCh-values, example	380-780 nm
Blank Line	-

7.1 Thickness Correction

If sample parameters of different materials with varying thickness (path length) are to be compared, it is necessary to transform the sample spectra to a nominal thickness.

Details of the pathlength correction are selected and entered in the **Thickness correction** window. The **Thickness correction** window allows you to activate and deactivate the correction status via the **Correction active**/**not active** buttons. See: *Calculations Window* 5-21

Once the thickness correction has been performed, the recalculated spectrum is displayed in the graph window together with the original sample spectrum. To distinguish it, the filename is extended with the string **~corrected**.

Note: *For spectral measurements of liquids in cells it is not necessary to consider the reflectance data, because the surface reflectance at the cuvette windows is compensated for with the baseline correction run. For this application therefore, set the reflectance value to the value "0".*

Tip: *A thickness correction is not feasible for reflectance spectra scanned as **%R**. A warning is given, if a method is to be saved with these options combined.*

All parameters for thickness correction – if activated – are elements of the method. The measured thickness can optionally be fixed or can be defined in the **Sample information** window.

Calculations for Sample Thickness Correction

The transmission spectrum of a non-turbid sample is determined by the pure material transmission values and the reflectance values at the two surfaces. The transmission values can be adapted to a nominal thickness according to the Beer-Lambert law. However, it is necessary to take the surface reflectance value into consideration; this must be specified by the user.

The software allows 3 different principles to be used to enter this value:

- Entry of a (wavelength-independent) reflectance value for a single surface reflection as **%R**, e.

g. 4 %R for a standard glass. A single value does not take into account the wavelength dependency of the reflectance. Generally, however, the accuracy of this procedure is sufficient, since the reflectance value only influences the calculation indirectly.

- When the reflectance value is not known, alternatively the (wavelength-independent) refractive index value can be entered. This value is used to calculate the reflectance value for normal incidence/unpolarized radiation. The software generates the reflectance value on this basis for normal incidence, according to Fresnel´s law for normal incidence of unpolarized light:

  $R = [(n-1) / (n+1)]^2$

  Nevertheless, this principle likewise does not account for the wavelength dependency of the reflectance value.

- Entry of a data file containing the single surface reflectance spectrum for the full wavelength range covered by the sample spectrum. This option assures highest accuracy for the thickness correction and is especially relevant if the sample spectrum spans a wide wavelength range, so that wavelength independency of the reflectance data cannot be assumed. This spectrum either can be scanned or can be calculated via the wavelength dependency of the refractive index and be entered manually.

Applied Norms and Conventions

The software applies the mathematical procedure as defined in the norms EN 410 and ISO 9050. It is valid only for homogenous samples, e.g. not for coated samples. Accidental negative transmittance values are calculated with their absolute and are set to negative after thickness adaptation. If the thickness correction calculation generates net transmission values larger 100 %T within the spectrum, ambiguous measurements or wrong correction entries are probable. In this case a warning is added to the sample description of the thickness corrected spectrum. In the above case and for single reflectance values of “0” within the applied reflectance spectrum, the reflectance calculations are dropped.

7.2 Weighting Factors

Many parameters calculated by the software are based on a weighted average (or convolution) calculation. This applies for the various transmission coefficients and protection factors. The weighting usually depicts the wavelength-dependent acting quantity $s(\lambda)$ (such as the incidence of radiation) and/or the wavelength-dependent material sensitivity $v(\lambda)$ (such as the skin sensitivity to UV radiation). The equation for the convolution with $T(\lambda)$ as the measured sample transmission data is:

$$\frac{\sum T(\lambda) \cdot s(\lambda) \cdot v(\lambda) \cdot \Delta\lambda}{\sum s(\lambda) \cdot v(\lambda) \cdot \Delta\lambda}$$

The results are typically given as a coefficient between 0 to 1 or as a percentage 0 – 100 %.

Solar protection values (SPF) generally are calculated as the reciprocal of the above weighted average.

7.3 Color Parameters

Color is of high relevance in everyday life. Thus, a large number of procedures have been generated to numerically quantify colors.

The classical procedures use a set of reference colors or colored reference solutions to describe the sample's color in respect to these; see: *Color Values* 7-12. Here, the individual color perception and partly also the viewing conditions remain unconsidered. Whereas many of these procedures are obsolete, a number of these still remain in use, e.g. to describe the quality of chemical solvents. The software allows generating some relevant color values by a mathematical evaluation of the sample's spectrum based on stored reference color data (i.e. without the subjective comparison by an operator).

The colorimetric procedures defined by CIE (Commission Internationale de l'Éclairage) are also based on the sample's spectrum in the visible spectrum range. They use a mathematical process that follows a standardized human viewing. As a result, generally a set of 3 figures evolves. See: *Colorimetric Evaluations* 7-5.

The set of 3 figures is also applied to quantify the color difference of a sample to a reference. See: *CIELab Color Difference Calculations* 7-8

Also, these data can be used to quantify the deviation to an ideal white (Whiteness index) and the strength of a yellow tint (Yellowness index). See: *Whiteness, Yellowness Index and Tint* 7-11.

The quantification of color influence of a transparent sample to the original color (Color rendering index, e.g. of a protection lens) is based on the CIE color calculations. These parameters are attributed to their respective norms.

7.3.1 Colorimetric Evaluations

Colorimetric evaluations are employed to describe the color of transparent and reflective samples in an objective way. As a starting point the transmission or reflection spectrum of the sample in the visible range is used. As a result a set of values is generated, which describes the color of a sample objectively and definitively (within measurements errors).

Calculation Procedures

The calculation process refers to an illumination and the human eye (observer) sensitivity. Since these parameters influence the resulting data triplet, they must be given for each set of color values.

Originating from CIE recommendations, the calculation procedures have found acceptance by many national and international standards, especially DIN EN ISO 11664 as one of the latest.

The software performs the color calculations according to these standards. The spectra must have been recorded on an absolute basis in the wavelength range of 360 – 830 nm. As reduced wavelength ranges 380 – 780 nm (extended range) and 400 - 700 nm are acceptable.
Calculations are based on data sets that contain the required observer and illuminant data with a 1 nm data interval. Highest precision is reached, if the sample spectrum also has been recorded with a 1 nm data interval. Other data intervals can be applied because the recorded data will be interpolated.
Both %R and %T spectra can be used.
Absorbance spectra are automatically transformed, if the ordinate designation is "A" (absorbance).

Typically, the results are given as a group, but also single result output can be defined.

Note: *Results from other systems that use a more coarse data base, can slightly deviate from the results of this software.*

The user may generate further data sets to extend the scope of illuminants, observers and wavelength ranges. Also, in the parameter definition file, output formats and wordings can be modified. See sections *Syntax of Parameter Definitions* 8-20 and *Color Calculations* 8-22.

Available Result Triplets

The color calculations generate 3 figures as an output. See *Syntax of Parameter Definitions* 8-20 .

• Tristimulus values	X, Y, Z	3-figure output (see below)
• Color coordinates	x, y, Y	3-figure output
• CIE color values Lab	L*, a*, b*	3-figure output
• CIE color values LCh	L*, C* (chroma), h* (hue angle)	3-figure output (see below)

With the tristimulus values it is also possible to generate the corresponding X0, Y0, Z0 values for the absolute white.
For the LCh output, also saturation S = C/L can optionally be generated.

Available Standardized Illuminants

- A light of a light bulb
- C daylight with cloudy sky (not provided with DIN EN ISO 11664)
- D65 daylight with clear sky and high sun

Available Observers/Angles of View

- 2 degrees focused viewing, CIE 1931
- 10 degrees broad-range viewing, CIE 1964

Calculations with further Illuminants

A further group of calculations is available for CIE Lab*-calculations with important illuminants. These are:

- Standard emission data of fluorescent lamps: F2 (cool white), F7 (broad range), F11 (TL84)

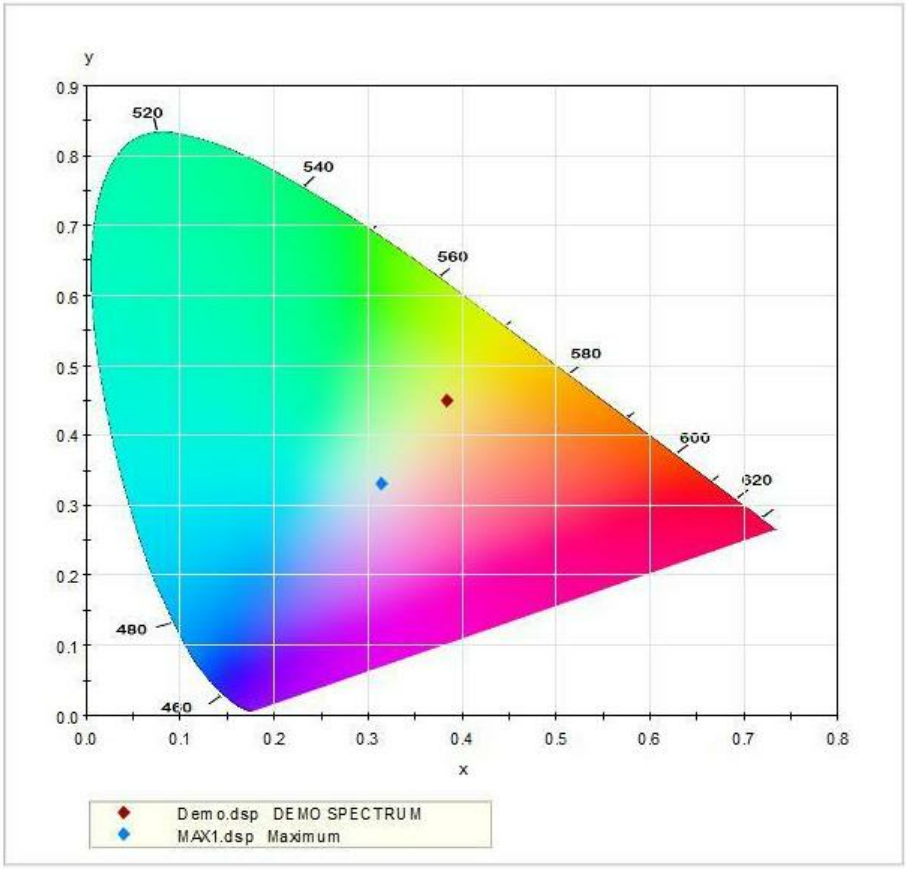
- Daylight simulators: D50, D55, D75

These calculations are based on data that are available in the 380-780 nm range with a 5 nm

data interval.

CIE 1931 Color Graph

The **Data Handling**/**Color Graph** function opens the **Print Preview** window to present a CIE 1931 color graph with the x,y color coordinates of the sample(s). Thus the graph allows checking the sample color visually. The full report can be printed or stored. See *Data Handling* 5-8 menu and *Print Preview* 5-6 window.



Spectrum: Demo.dsp DEMO SPECTRUM
Chrom. Coordinates xyY (Ill. D65/10 deg obs./380-780nm) x:0,384 y:0,451 Y: 15,9

Spectrum: MAX1.dsp Maximum
Chrom. Coordinates xyY (Ill. D65/10 deg obs./380-780nm) x:0,314 y:0,331 Y: 40,0

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Note: *Technically speaking the graph is only valid for CIE 1931 (2 deg observer) calculations. However, deviations typically are small.*

In order to automatically generate the report after a measurement, copy the *Color graph CIE 1931_Lxx_abxx.sc.rpx* and the *Color graph CIE 1931.oc2* template files from the **Data** directory to the **Methods** directory and rename them to the name of the employed method. See *Report Configuration* 8-35.

Literature

Details about colorimetric theory and practice are found in various textbooks and websites, e.g.:

G. Wyszecki, W.S. Stiles
Color Science: Concepts and Methods, Quantitative Data and Formulae
Wiley-Interscience 1982

7.3.2 Color Difference

The color difference of a sample to a reference is determined to quantify small color tolerances of colors. The color difference value is calculated from the color values of both the sample and the reference. In literature, a large number of proposed procedures is described. This software offers the following options:

CIE Lab	Color difference according to CIE 1976, e.g. DIN 6174
CMC (2:1), CMC (1:1)	Color difference defined by *Colour Measurement Committee of the Society of Dyers and Colourists in the British Standards Institution (BSI)* (1984)
CIEDE2000 (1:1:1)	Color difference according to CIE 2000, as defined e.g. by DIN EN ISO 11664-6

All available calculations are based on the L*a*b*, resp. L*C*h* color space as defined by CIE in 1976. CMC and CIEDE2000 color difference calculations additionally apply correction factors to improve color uniformity.

For CMC color difference calculations, the influences of lightness and chroma are weighted; the software offers the common weighting 2:1 and 1:1. Additional definitions with other weighting can be added, see below. With CIEDE2000, also hue can be weighted.

In the norms the illumination and the observer are not specified. This means that these parameters must be given with the color difference results. The software offers the standard setting illuminant D65 and 10 deg observer in the standard wavelength range 400 - 700 nm, resp. 380 - 780 nm for CIEDE2000. Parameter definitions with other illuminants/observer may be added. It is also possible to utilize self-defined sources, see section *Color and Color Difference Calculations* 8-22.

The total color difference is described by the value $\triangle E$, which usually is used as the test value. Additionally it is possible to split up the contributions:

$\triangle L^*$	Lightness contribution
$\triangle C^*$	Chroma contribution
$\triangle H^*$	Hue contribution
$\triangle a^*$	Difference on red/green scale (not with CMC)
$\triangle b^*$	Difference yellow/blue scale (not with CMC)

The software calculates the overall color difference and the 3 or 5 contributions. Accordingly, the report output includes a set of 4 or 6 figures.
As a reference, either a set of Lab^* values, XYZ values or a spectrum of a reference sample can be given, see below.

Note: *Make sure that the reference spectrum covers the required spectral range, which is normally 400 – 700 nm or 380 - 780 nm for CIEDE2000.*

Note: *Make sure that the reference spectrum/data are measured under the same conditions as the sample spectrum and that the reference $L^*a^*b^*$ values are calculated with the same illuminant/ observer as used for the color difference calculation.*

Use the **Color Difference Setup** function of the **Calculations** window to modify, add or delete color difference calculation parameters; see *Calculations Window* 5-21.

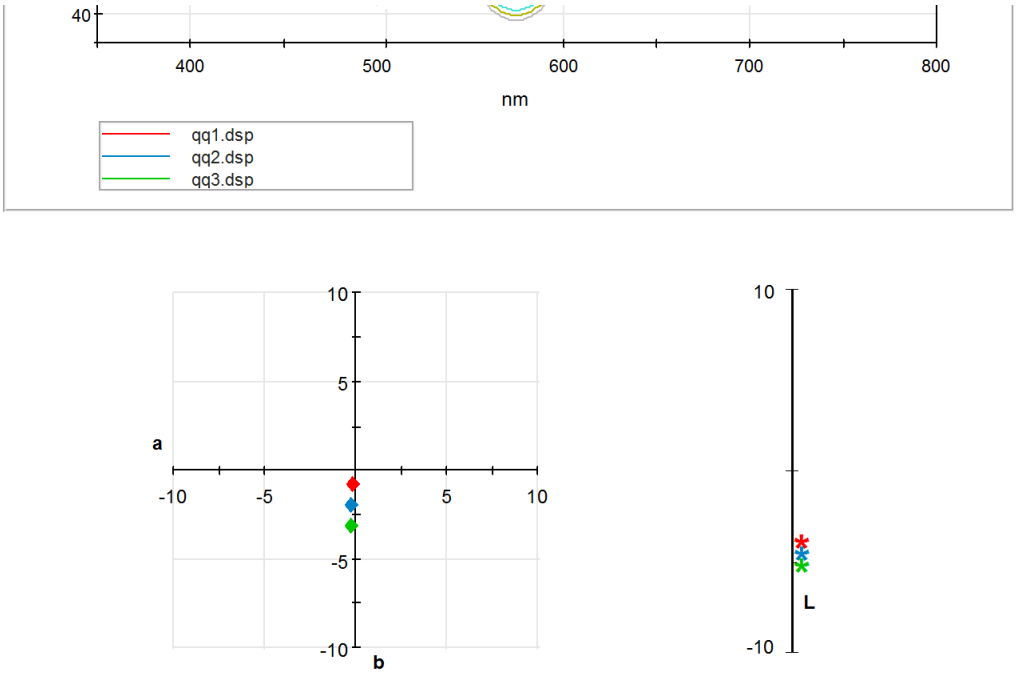
CIE Lab Color Difference Graph

When calculating color differences, a visual presentation of the results is common. Typically, a Da*/Db* graph and a DL* graph is employed. Use the **Data Handling/Color Difference G raph_Lxx_abxx** (xx = 5 or 15) function to generate a **Print Preview** report with implemented color difference graph. See *Data Handling* 5-8 menu and *Print Preview* 5-6 window.

The function generates a report of the results with the color difference graph included, if a CIE Lab* color difference evaluation is part of the results in the **Results** area.

Note: *If you need a different scaling of the graphs, make a copy of a Graph_Lxx_abxx.sc.rpx and rename it. The figures xx within the function name define the scaling of the L- and the ab-axes of the color difference graph.*

Important: The CIE Lab Color difference graph is taken from the first CIE Lab* color difference evaluation of a sample. Additional color difference results cannot be presented graphically. Also, CMC or DECIE2000 color results cannot be presented.
However, results of a series of measurements are presented in the graph.



Additional CIELab Color Difference Graph with 10 units scaling

In order to automatically generate the report after a measurement, copy the *Color Difference*

Graph_Lxx_abxx.sc.rpx and the *Color Difference Graph_ab.oc2* template files from the **Data** directory to the **Methods** directory and rename them to the name of the employed method. See *Report Configuration* 8-35.

7.3.3 Dominant Wavelength; Excitation Purity

The dominant wavelength is the wavelength of the pure spectral color that is near to the sample's color. The value can be taken as a measure of hue. Together with purity and brightness, the values are a way to describe colors that is not so common anymore. However, it is sometimes preferred, if the hue is mostly pure.

The dominant wavelength is detected graphically within the CIE color space chromaticity graph (horseshoe diagram): The outer curved enveloping boundary (the spectral locus) of the diagram is established by the pure spectral colors; each color point is represented by a wavelength. The straight line from the respective white point of the diagram to the color point of the sample is extrapolated to the diagram's envelope curve. The wavelength corresponding to the point of intersection is designated the dominant wavelength of the sample's color. If however, the extrapolated straight line does not intersect with the curved envelope, but with the straight line of purples (the straight connection of the red and blue corners), a dominant wavelength cannot be generated. Instead, typically the complimentary wavelength (see below) is output with a negative sign.

For determining the dominant wavelength an illuminant and an observer must be selected.

The value of the dominant wavelength and its related parameters can have lower accuracy, if the dominant wavelength is near to the ends of the diagram's envelope curve, i.e. < 450 nm or > 600 nm. Specifically for the 2 deg observer a dominant wavelength > 700 nm cannot be given, because all wavelengths are on the same spot. Also, results for near-white colors (chromaticity coordinates near white point) can have a low accuracy because of the far extrapolation.

In addition to the dominant wavelength further related parameters are output in a bracket. If this output is unwanted, it can be removed by editing the parameter definition file.

- The complementary wavelength C*ompl* is determined as the wavelength on the diagram's envelop, where an extrapolation from the color point over the white point intersects; this is an extrapolation as the above for the dominant wavelength, but to the opposite direction. If the dominat wavelength is set to the negative complemtary wavelength, the complementary wavelength itself is set to 0.0 nm.

- The excitation purity *Pe* can be used as a measure for saturation. It is calculated as the ratio of the distance from the white point to the sample and the distance from the white point to the dominant wavelength. Distances are taken on the extrapolated straight line used for determining the dominant wavelength. Pure spectral colors have a purity of excitation of 1 or 100%. If the straight line does not intersect the spectral locus, the intersection to the line of purples is applied accordingly.

- An alternative measure is the colorimetric purity *Pc*. This value is based on the excitation purity. The value is calculated as described in *Steven K. Shevell: The Science of Colors (Opt. Soc. Am. 2003)*. The formula does not apply the complementary wavelength, if a dominant wavelength cannot be defined, as described with older literature.

7.3.4 Whiteness, Yellowness Index and Tint

Whiteness, Yellowness Index and Tint combine the XYZ or xyY values to describe the named characteristic with a single figure.

Whiteness Index

The Whiteness Index (WI) describes the degree of similarity to the ideal white color or the absence of colored or gray tones for a sample. A large number of procedures and calculations are described in the literature. Ganz gives an excellent overview about the topic (Appl. Opt. 18, 1073–1079 (1979)).

One of calculations offered, follows CIE recommendation with a neutral preference:

$$WI = Y - 800 \cdot (x - x_0) - 1700 \cdot (y - y_0)$$

For the WI (Ganz) the same formula with the coefficients 1869.3 and 3695.2 is used.

Y and x/y refer to the illuminant D65 with a 10 degree observer for measurements in the range of 400 to 700 nm.

The Whiteness Index of ASTM E313-05 is also based on the above calculation formula, but offers different illuminants/observers.

Tint Index

The Tint-Index (TI) measures the amount of tint of a sample. ASTM E1313-05 gives the following calculation

$$TI = T_X \cdot (x_n - x) - T_y \cdot (y_n - y)$$

The factors T_X and T_Y vary according to the illuminant/observer.

Yellowness Index

The Yellowness Index (YI) quantifies the amount of yellowness of a sample, e.g. generated by bleaching. ASTM E1313-05 gives the following calculation

$$YI = 100 \cdot (C_X \cdot X - C_Z \cdot Z) / Y$$

The factors C_X and C_Z vary according to the illuminant/observer. The older ASTM D1925-62, which has been made obsolete, uses the factors $C_x = 1.28$ und $C_z = 1.06$ with the tristimulus values for C/2° (CIE 1931).

7.3.5 Color Values

Technical liquids often have a slight yellow color due to contamination or decomposition products. The strength of this color is an important criterion of quality and typically a measure of purity. Whereas traditionally, color classification for this type of sample is performed by visual comparison of the sample with yellow reference solutions in defined vessels, this software allows to generate the data without refernces. The procedures are described by norms.

Table: International Norms Concerning Color Values

Norm	Description	Comments
ASTM D 1209-00	Test Method for Color of Clear Liquids	Platinum-Cobalt Scale (Pt-Co)
BS 5339:76 (1993)	Measurement of Color on Hazen Units	Platinum-Cobalt Scale (Pt-Co)
DIN 53409 (1997)	Determination of Hazen Color Data	APHA procedure
EN ISO 6271-1 (2004)	Clear liquids – Estimation of color by the platinum-cobalt scale	Evaluation by visual method
EN ISO 6271-2 (2002)	Clear liquids – Estimation of color by the platinum-cobalt scale	Spectrophotometric Method
DIN EN ISO 4630-1 (2005-3)	Clear liquids – Estimation of color by the Gardner color scale	Evaluation by visual method
DIN EN ISO 4630-2 (2005-3)	Clear liquids – Estimation of color by the Gardner color scale	Spectrophotometric Method
ASTM D 1544-98	Test Method for Color of Transparent Liquids	Gardner Color Scale
ASTM D 6166-97 (2003)	Test Method for Color of Naval Stores and Related Products	Instrumental Determination of Gardner Color
DIN 6162 (1981)	Determination of Iodine Color Number	
ASTM D 6045 (2009)	Standard Test Method for Color of Petroleum Products by the Automatic Tristimulus Method	Saybolt color and ASTM color forr petrochemical products

Further Information on Calculated Color Values

The calculated color values are within the following scales:

- *Pt-Co/APHA-/Hazen* 7-14
- *Gardner* 7-16
- *Iodine* 7-18
- *Saybolt and ASTM* 7-21

Important Characteristics of the Color Value Determination

Whereas the Iodine Color Number is applied for stronger colored samples, the Pt-Co/APHA color value is mainly used for weakly colored samples. The Gardner color scale tries to cover a wider range by employing 2 different color solutions. Apart from that the mentioned color scales have been selectively established in different application areas.

As in other ranges of color determinations, there is a trend to replace the subjective and costly procedures by an objective, measuring procedure. Another problem, e.g. for the Pt-Co/APHA color scale is that the reference solutions are not stable when used regularly.

ISO/DIS 6271-2 and 4630-2 are designated to describe a spectrophotometric method, but they mainly mention that a suitable instrument is to be used. ISO/DIS 4630-2 additionally describes a mathematical procedure, which is used by the software.

An objective procedure is based on the sample spectrum in the visible spectral range, which is typically 380 to 780 nm. These data are taken to calculate integral color coordinates, which are the basis for comparison to the stored data of the reference solutions. Therefore it is not necessary to handle reference solutions. As a result, numerical data are generated, which can be documented and investigated by procedures of statistics.

Anyhow it is recommended to check the procedures with commercial reference solutions for a validation of the process.

Correct execution of the baseline compensation run and removal of sample turbidity are very important for a correct determination of small color values, see below.

Configuration of Color Evaluations

Typically, the generated color results consists of two figures, the actual value and a figure describing the color deviations, see below.

For all described color determinations, it is possible to change the order of parameters, the wording of the text messages and other details of the output. This is done by editing the parameter definition file **VL_ColorCalc.dta**, see also the corresponding section. See: *Data Formats and Import/Export* 9-1

Color Deviations

Any uni-dimension color scale will fail, when the color of the sample deviates substantially from the color of the reference solution. In this case erroneous and misleading results can be generated; despite the fact that the employed integral calculations are less sensitive to color deviations than the more simple single wavelength procedures. Probably an experienced user will be superior to compensate for color deviations; however any user will do that on his personal basis and experiences.

To support the user with the procedure, any parameter (not Saybolt/ASTM) also offers an option for estimating the degree of color deviation.

General Practical Hints

Perform the baseline compensation run with the same or a similar cell (same type and material)

under the same instrument settings as the sample measurement. In a double beam spectrophotometer, the reference position can be left free. The spectral range must be at least 380 to 780 nm. The data interval can be chosen freely, however data intervals of 10 nm or higher will deteriorate accuracy.

For weakly colored samples, the baseline compensation should be run any 1 or 2 hours to compensate for the drift of the instrument.

Make sure the cell has been filled without bubbles. When changing from an organic solvent to water or vice versa, make sure that the cell has been dried completely. Plastic cells (single use cells) are not recommended for weakly colored samples. This is because the homogeneity of the cells typically is insufficient.

Especially when working with viscous materials there is a problem of schlieren or streaks within the liquid. Also air bubbles may be included, that do not evade. These effects will scatter light and will result in lower transmission values, thus generating apparent higher color values. Make sure that you use proper cuvette filling techniques and that you thermostat the sample.

The same effect can be generated by particles and turbidity in the sample. Though this does as well affect the visual impression, the influence on the spectrophotometer readings will be different. Furthermore the effect will be dependent on the specific instrument construction. DIN 6162 and ISO/DIS 4630 recommend a filtering of the sample anyhow. If it should not be possible to remove turbidity, another instrument layout, e.g. an integrating sphere accessory, should be applied.

Norm EN 1557

If for any reason, the described color determinations should not be adequate, as well the procedure of EN 1557 (1997-03) (Surface active agents. Colorimetric characterization of optically clear colored liquids (products) as X, Y, Z tristimulus values in transmission) could be an interesting alternative. The respective evaluations are available in the software. See: *Colorimetric Calculations* 7-5

Pt-Co/APHA/Hazen

The colors of technical liquids are frequently classified according to the Pt-Co/APHA-/Hazen color scale. These three designations are commonly used in different application areas, but they are all based on identical procedures. According to ISO/DIS 6271 the name Pt-Co color scale is preferable.

According to a proposal by A. Hazen in 1892, the Pt-Co-/APHA-/Hazen color scale uses an acidic solution of potassium hexachloro-platinate(IV) and cobalt(II) chloride. The reference solutions are designated according to their platinum content in mg/L in the range 0 to 500. The solutions can be also obtained from commercial suppliers.

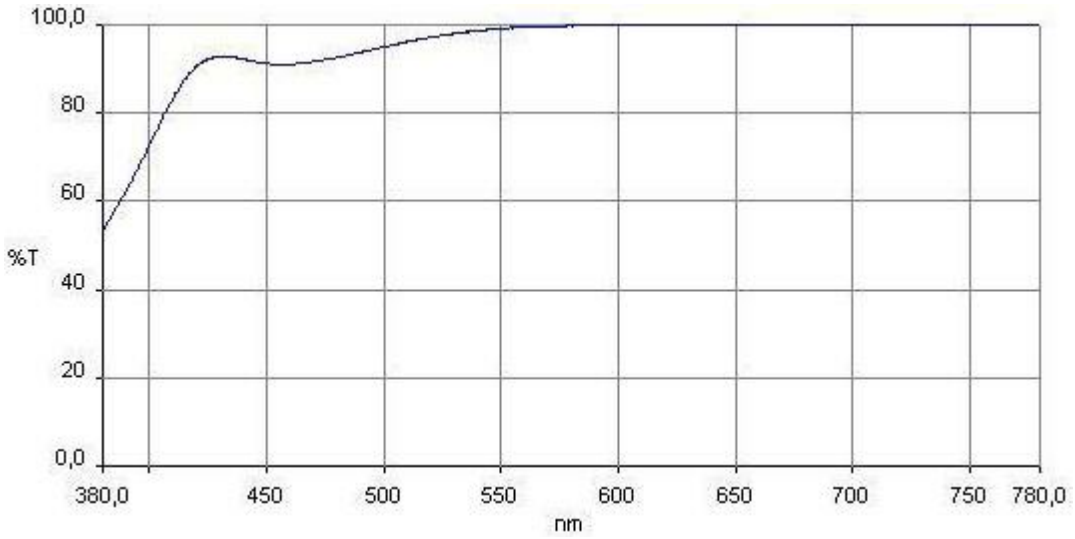


Figure: Spectrum of a Pt-Co reference solution (APHA color value 100) in a 1 cm cell

Typical application areas of the Pt-Co-/APHA-/Hazen color scale include polymer additives, water and wastewater, resin solutions, and solvents such as hexane, glycerol, methanol, mineral oils, etc. The recommendation of this procedure by the American Public Health Agency (APHA) has established the respective naming.

The software includes an appropriate algorithm, which is based on a unique calibration of the Pt/Co reference solutions. The calibration curve is included in the software. Using this calibration curve, the sample's APHA-/Hazen value is calculated from a color value obtained for the sample spectrum. Calibration data are included for 1 cm, 5 cm, and 10 cm cells, so that very light coloration can also be determined. The detection limit can be estimated to 0.5 units. This gradation is much finer than recommended by DIN 53409 for example, which describes the rounding of the result to the nearest ten.

Color Deviations

As with the other one-dimensional color scales, deviations of the color tone between sample and references will result in an uncertainty of estimation. Comparing colorless or red, green or blue colored samples can give erroneous or meaningless results, which will no longer correlate to visual judgments.

For each result, the software calculates the hue angle, which allows an estimation of the color difference to be made. The hue angle can cover the range of 0 to 360 deg. The reference solutions have a typical value in the range of 100 deg with a decrease towards stronger colored samples. Sample solutions should not deviate too markedly.

The user should fix a tolerable range for the hue angle according to visual estimations. Note that the tolerance must be larger at smaller color values due to the increased influence of systematic and statistical errors of the spectrometric measurement. Typical measured values are:

Pt-Co color value	Hue angle 1 cm cell	Hue angle 10 cm cell
5	102	100.8
15	100.5	100
30	100	99

Pt-Co color value	Hue angle 1 cm cell	Hue angle 10 cm cell
60	99.9	97.8
100	99.6	95.9
200	99.2	

Practical Hints

With small Pt-Co color values transmission values of 98 to 100 %T have to be measured correctly. Therefore the correct and careful performance of the baseline correction is of overall importance. especially for weakly colored samples. Execute the baseline correction run with the colorless pure component or with the solvent, when a dissolved component is to be measured. Baseline correction material and sample should have the same temperature. When the pure component used for baseline correction is actually not colorless, the results will be too small for the samples.

If the pure component is not available in the required purity, a solvent with a similar refractive index can be used as an alternative. This however will reduce the possible result accuracy.

Depending on the typical spectrophotometer drift, it will be necessary to repeat the baseline correction any 1 or 2 hours.

Please note that with nearly colorless samples, even negative values can result – either due to systematical and statistical errors of the spectrometric measurement or due to color deviations.

See also: *General Practical Hints* 7-13

Gardner Color Values

Just as the other described color scales, the Gardner scale also aims to estimate the color of yellow to brownish liquids. The application area of his scale is mainly binding agents and thickeners for paints. The Gardner scale is designed to cover a wide range of color intensities, but does not consider very weakly colored samples.

The procedure for visual inspection is described in DIN EN ISO 4630-1. The software uses the procedure as described by DIN EN ISO 4630-2. The norm is nearly identical to ASTM D 1544.

The color scale uses 8 solutions of potassium-hexachloroplatinate(IV) and 10 solutions of Co(II) Cl_2/Fe(III)Cl_3 as stronger colored references.

The norm reproduces the color coordinates for all 18 reference solutions (illuminant C, 2 deg observer) and describes an algorithm to determine the Gardner color value from these and the xyY color coordinates of a sample. The result is the Gardner color value with one fractional digit. The integer and fractional digits are derived in two separate steps. The resulting Gardner color value is the sum of the two sections.

When the sample color deviates substantially from the color of the similar reference, the fractional digit calculation may give a value above or below the expected range of 0 to 1. The norm does not give advice for such a case.

The additional parameter *Gardner color check* will test the level of the fractional digit result. If the range is between 0 and 1, the message *Sample is within color scale* will be output. Otherwise the message *Sample is outside color scale* will be given. Thus the user has an option to estimate the color deviation of the sample. It may be become necessary to adapt the tolerance

according to practical experience.

Another calculation parameter allows comparing the result of Gardner color value to a given limit. The output is given as a text. The example parameter compares the Gardner color value to the value of 5. Other settings can be done by editing the parameter definition file. See: *Adapting the Evaluation Parameters* 8-17.

Out of Range Gardner Color Values

The Gardner color scale is limited to values in the range of 1 - 18. Colors with a Gardner value below 1 and above 18 cannot be derived from the algorithm and they are explicitly undefined. The software uses a suitable expansion of the algorithm applying interpolated data for a hypothetical Gardner color values 0 and 19. However note that Gardner color values below 1 and 18 are not compliant to the norm.

Gardner Color Values smaller 1

The software defines a white point with Gardner color 0. Thus Gardner color values below 1 and even small negative values can be output. Negative values may derive from minor instrument or handling errors. In analogy to the logical decision described above, the parameter definition file can be extended to allow a warning output for Gardner results <1.

Gardner Color Values above 18

The software additionally defines a hypothetical point for Gardner color value 19. Thus is becomes possible to calculate Gardner values that have an integer section of 18. Accordingly, Gardner color values slightly higher or lower than 18 can be generated. Values above the limit are output as 99.

Practical Hints

The measurement is done in 1 cm cells in the wavelength range of 380 to 780 nm. For baseline correction the colorless pure component or the solvent is used.
The correct and careful performance of the baseline correction is of overall importance, especially for weakly colored samples. Execute the baseline correction run with the colorless pure component or with the solvent, when a dissolved component is to be measured. Baseline correction material and sample should have the same temperature.

When the pure component used for baseline correction is actually not colorless, result will be too small for the samples. If the pure component is not available in the necessary purity, a solvent with a similar refractive index can be used as an alternative. This however will reduce the possible result accuracy. See also: *General Practical Hints* 7-13

Iodine Color Values

The visual determination of the iodine color value is described in DIN 6162. The figure serves to describe “the color depth of clear liquids, e.g. solvents, softening agents, resins, oils and fatty acids, the color of which is similar to that of a potassium-iodine solution".

The iodine color value is given as “the amount of iodine [mg] in 100 ml of an aqueous solution, which has the same color depth as the sample compared with the same thickness”. The norm describes a visual comparison.

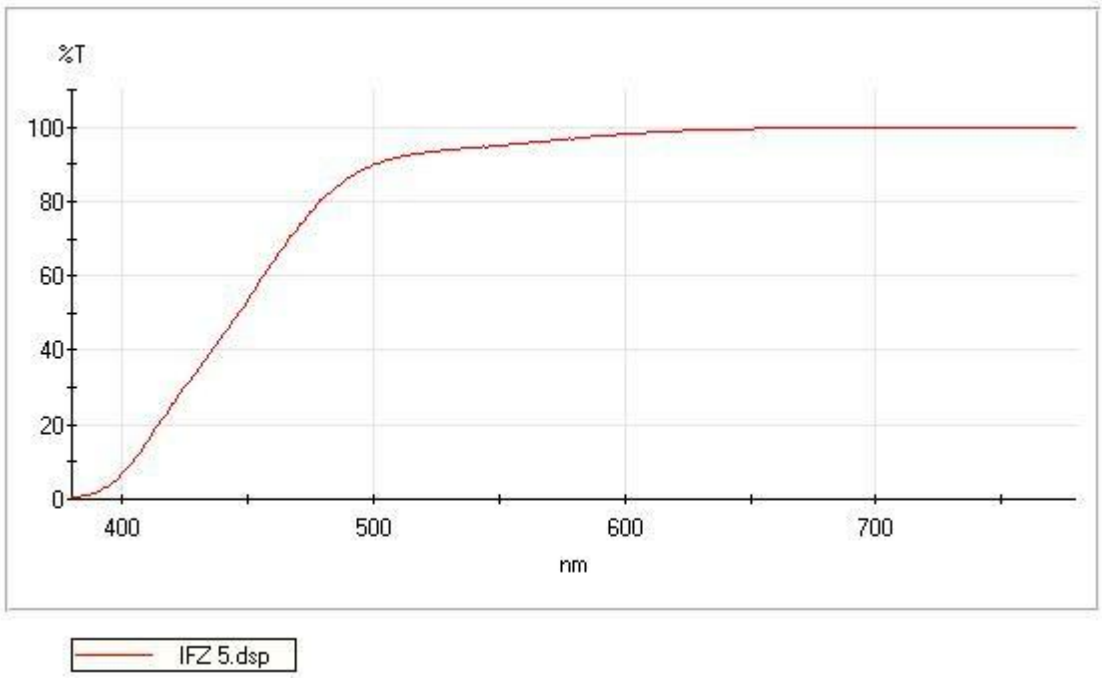


Figure: Spectrum of an iodine reference solution (color value 5)

The software uses the spectrum of the sample measured in reference to pure water. The wavelength range is 380 to 780 nm and the cell path length is 1 cm. The spectrum is used to derive a specific color value, which is compared to the stored reference values. As a result iodine color values in the range of 0 to 50 units are output. Thus the procedure imitates the visual comparison by objective measurement techniques and provides a comprehensible and documented determination of the iodine color value.

Working Range

DIN 6162 designates iodine color values smaller than 1 as uncertain and recommends to use the Pt-Co color value instead. Experience shows that the herein described determination process used by the software is able to determine iodine color values down to 0.2 units.

Note: *For nearly colorless samples, possibly resulting negative values – either due to systematical and statistical errors of the spectrometric measurement or due to color deviations – are set to “0”.*

DIN 6162 lists a reference solution of 50 mg/100 ml iodine as the strongest reference solution. Samples colored as strongly as this are typically rare. It is recommended, to critically observe samples with an iodine color value higher 30, because substantial errors can occur. Results larger than 50 are set to 99.9.

Color Deviations

The norm expresses that “the method must not be used with larger deviations of the color of the sample compared to the color of the references. As with the other one-dimensional color scales, deviations of the color tone between sample and references will result in an uncertainty of estimation. Comparing colorless or red, green or blue colored samples can give erroneous or meaningless results, which will no longer correlate to visual judgments.

For each result, the software calculates the hue angle, which allows an estimation of the color difference to be made. The hue angle can cover the range of 0 to 360 deg. The reference solutions have a typical range of 113 to 95. Sample solutions should not deviate too markedly from the values given in the table below.

Iodine color value	Hue angle
0,5	113
1	113
2	112
5	109
10	105
20	100
30	95

Practical Hints

Measurement is done in 1 cm cells with a wavelength range of min. 380 to 780 nm. The baseline correction run is done with a cell filled with pure water without bubbles. In a double-beam spectrometer the reference beam position can be left empty.

Measure the sample in the same or a similar cell (same type and material) under the same instrument settings as the baseline correction run. The data interval can be chosen freely, however data intervals of 10 nm or higher will deteriorate accuracy. When changing from an organic solvent to water or vice versa, make sure that the cell has been dried completely.

When the refractive index of the sample is substantially different to that of water, the resulting color values may be too small or too high. In this case it is superior to do the baseline correction run with the pure component or the solvent. See also: *General Practical Hints* 7-13

EP Color Examination

The European Pharmacopoeia and related national pharmacopoeias describe the color examination of pharmaceutical raw materials. The principle uses five series of stable colored solutions, each of which is diluted to 7 or 9 shades. The color of a sample is examined by visual comparison to one or more of these references.

Advantages of Spectrometric Color Examination

Visual comparisons nowadays are generally looked upon skeptically, because they are subject to individual conditions. Illumination, surrounding colors as well as personal differences and feelings will affect color examinations. Furthermore, individual visual inspections may not be reproducible and cannot be quantified.

On the other hand the color of a (non-fluorescent) sample is strictly defined by the sample transmission spectrum in the visible spectral range (400 to 700 nm). Such spectra can be

scanned easily and reliably with a standard UV/Vis spectrophotometer and saved on a PC in digital form. However, a spectrum typically comprises up to several hundred data points and such large data sets are not easy to overview.

The advantages of the spectroscopic procedure are that an objective value is applied, which can be statistically treated, and that the reference solutions must not be prepared for each measurement.

Performing Spectroscopic EP-Color Examination

Because of the problems arising from visual color examination, it has been suggested to perform the described color inspection objectively by processing the recorded sample and reference spectra mathematically. This requires that the necessary reference spectra be scanned once and used as the basis for the color inspection. Anton proposed an appropriate calculation scheme in his thesis (1). This scheme calculates a characteristic color value, which is almost linear to the dye concentration. Thus it is simple to use this single value for comparing the color depth of the sample to the stored data of the reference solution.

***Note**: It must not be overlooked that the color comparison is only valid, if the tonality of the sample is equivalent to that of the applied reference solution. Differences in tonality can result in a misleading rating.*

(1) E. Anton: Validierung der Farbmetrik und Untersuchungen zur Aufnahme der instrumentellen Trübungsmessung in das Arzneibuch, Würzburg (Germany) 2000

Results Output

The result of the calculation is a decision as required by DAB/EP, e.g.:

C=2.81; dh=1.12 Sample is more strongly colored than reference B6 (C=2.62)

C is the sample color value, which can be compared to the given color value of the reference solution. Additionally the hue difference is output. It allows estimating the difference in color tone between sample and reference solution.

Applied Reference Data

The software contains all characteristic values of the reference solutions described in DAB/EP in 1 cm cells:

Brown	B5 – B9	
Brown-yellow	BG4 –BG7	(equivalent to BY)
Yellow	G4 – G7	(equivalent to Y)
Green-yellow	GG4 – GG7	(equivalent to GY)
Red	R4-R7	

Additionally also evaluation in reference to the weaker colored solutions can be done in 5 cm cells.

Saybolt/ASTM Color values

The color of petrochemical products like gasoline, diesel fuel, kerosene, wax, etc. is an important criterion for example for product quality.The color may indicate the product's purity and the degree of refining. Color can also be a rough measure of additives in a product. With used petrochemical products, the color can be used as a measure for product oxidation and contaminations. Mainly, this results in a yellow to brown or reddish brown color.

Saybolt/ASTM Color Values with ASTM D6045

Traditionally, the color of petrochemical products is tested via visual inspection in a dedicated optical apparatus in comparison to liquid standards. These procedures are defined by ASTM G159 (Saybolt color) and ASTM D1500 (ASTM color). The numerical rage for Saybolt color is -16 (strongly colored) up to 30 (weakly colored); the range for ASTM colors is 0,5 to 8 (strongly colored). Generally, the Saybolt color scale is applied for weakly colored samples, whereas the ASTM color scale is used for stronger colors.

These procedures are tedious and they lack objectiveness. The newer norm ASTM D6045 (Standard Test Method for Color of Petroleum Products by the Automatic Tristimulus Method) of the year 2009 describes a procedure that calculates both Saybolt and ASTM color values from the sample's CIE color data (X, Y and Z). See *Colorometric Calculations* 7-5.

Cell Thickness for Saybolt and ASTM Color Determination

Both calculation paths use a sample's colorimetric parameter calibrated against the values of standards. For **Saybolt color** values, a cell thickness of 10 cm is used; for **ASTM color** values a cell thickness of 33 mm is used for the calibration. For these conditions, the norm lists the calibration data. The software uses these calibration data. Thus it is possible to generate the Saybolt and ASTM color values directly from the sample's transmission in the 380-780 nm wavelength range. If you have established your specific calibration data, these can be introduced by editing the parameter definition file. See *Adapting evaluation parameters* 8-17.

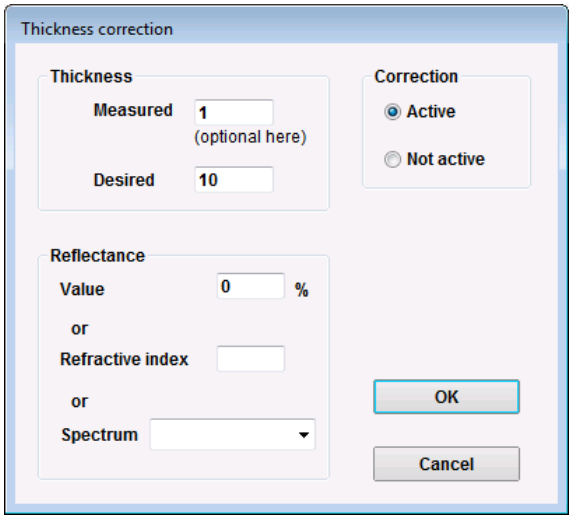


Figure: Setting for Thickness correction for a Saybolt color evaluation

The software allows evaluating spectra that have been recorded with cell path lengths other than defined by the norm. For that a **Thickness correction** must be defined in the method; see

Thickness correction 7-3. The **Desired** path length is as given by the norm, the **Measured** path length actually applied. "0" (zero) must be entered as the **Reflectance Value**.

Note: *The **Thickness correction** is performed with the measured spectrum and therefore also applies to other evaluations that are done correspondingly. So it is not possible to do a **Saybolt** evaluation with thickness correction together with for example a Pt/Co evaluation in one report.*

7.3.6 Color Wine and Juice

White, 'blanc de noirs' and red wines differ in their colors in a wide range, depending on the grapes, the maturity and their treatment. Certain color characteristics stand for quality and originality. The standard CIE color description procedures can be applied after measuring the transmission sample spectrum (red wines after dilution or with reduced path length). However in wine industry, still the older, single-wavelength color description prevails. xyY and Lab-data are becoming popular slowly.

Red wine typically has an absorbance maximum around 500 nm and a minimum around 420 nm. As originally proposed by Sudraud (1958), absorbance readings of these spectral details are taken at 420 and at 520 nm: The sum of the readings is named color intensity or density, the ratio A420 / A520 is named the tonality, hue or tint. Glories (adapted by OIV/ ORGANISATION INTERNATIONALE DE LA VIGNE ET DU VIN) additionally adds the absorbance at 620 nm. Other authors try to describe the color of red wine by its anthocyanides contents quantified by its peak absorbance in the range of 510 – 540 nm. This value can be corrected by a scattering reading at 700 nm.

An attempt to describe the level of the blue, white and red contributions is to ratio the readings at 420/520/620 to the sum of these readings (Color Percentages).

White wines do not have specific absorbance characteristics. So the absorbance at 420 nm is taken as the color intensity.

Further spectrometric calculations include chemical treatments of samples and a calculation with readings of the modified and the untreated sample. As examples the difference of absorbance at 520 nm and the calculation of the Polymeric Color Ratio are included.

The software offers the following parameters. Note that the calculation expressions expect %T spectra.

- Abs (420 nm)
- Abs (520 nm)
- Abs (620 nm)
- Tonality Sudraud (420/520 nm)
- Color Intensity Glories (420/520/620 nm)
- Color Intensity red. (420/520 nm)
- Peak Abs (Peak 510-540 nm)
- Peak Abs haze corr. (Peak 510-540 nm/700 nm)
- Color Intensity red./peak haze corr. (420/Peak 510-540 nm/700 nm)
- Color Percentages yellow
- Color Percentages red
- Color Percentages blue
- Diff Abs (520 nm) to proc. spectrum
- Polymeric Color Ratio

Samples are typically measured in 1 cm cells after filtration. Red wines must be diluted up to 1:10 or be measured with a small path length cell.

7.4 Calculations, Decisions and Classifications

Besides the predefined calculation parameters the software also offers options to define calculation, decision and classification expressions. These can be applied to spectral data extracted from the spectrum (single value, peak value/position, area or slope) or to results as generated by a predefined parameter calculation.

The list of parameters contains a some calculation expressions in the Wine Color section, which can serve as a pattern. Also, some calculation expressions are marked as "example" that can be applied with user defined values.

Further information about the syntax is given in other sections. See *Calculation Expressions* 8-23 and *Syntax of Parameter Definitions* 8-18. Also contact ***ascanis*** directly for further support.

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8 Software Configurations

The software can be configured in various ways.

- Some options (e.g. print format or data and method directory) are selected with the user interface. These settings are automatically stored within the software configuration file **VL _ColorCalc.ini**.

Other settings will be changed only once or rarely:

- Some settings are accessible by editing the configuration file with the Windows Notepad. See: *Options in the Configuration File* 8-3
- Other settings defined only once or rarely can be modified by extending the software startup command. See: *Options in the Software Start Line* 8-7

Basic and temporary software settings are contained in 3 configuration files.

	Relevance	**Location**
VL_ColorCalc 8-2 User.ini 8-2	User-specific configurations	Windows Vista/7: C:\Users\<user name>\AppData \Roaming\<software name> Other: C:\Documents and Settings\<user name>\ Application Data\<software name>
VL_ColorCalc.ini 8-3	Measurement and instrument settings	Data directory as defined in installation
VL_ColorCalc.cfg 8-2	Basic software settings	Program directory as defined in installation

Note: *Before modifying the configuration file make sure to have a copy. Also, close the software before editing the configuration file. The software will only adapt to the new setting, when re-started.*

Important: *For reflectance measurements, the required data for for the white and dark correction must be adapted to the spectrophotometer system in use. See: Reflectance Measurements* 8-9.

It is possible to adapt the report header, see *Adapting the Report Header* 8-11.

Offline Operation of Standard Version

The software is optionally offered in a specific offline version. Also the standard version can be set to an offline mode. With both options, stored spectra of various formats can be loaded and evaluated with the **Recalculate** function. See: *Data Formats and Import/Export* 9-1 and *Recalculate* 5-33.

If you wish to use the standard software offline only, please select the following setting:

1. Select the command **Preferences** in the **Options** menu.
2. Select **None** for the **COM**-port.

This will prevent error messages due to the missing spectrophotometer. The software will not try to access the spectrophotometer and does not activate or show instrument related parameters.

***Tip**: The **Save automatically** option is not active in offline operation.*

8.1 General and User Configuration

Configuration options that cannot be modified or that are rarely modified are summarized in a user specific and a general configuration file.

The User specific Configuration File

A user-specific configuration file is setup for each user automatically. This file is located as **VL_ColorCalcUser.ini** in the user specific directory area and thus is valid only for the respective user.

The file holds information like the previously used method, the previously used window size and the 25 recent **Operator** names. Also the information of the *MethodLink* und *URAStepper* routines are held in this file. The file is refreshed each time, the software is terminated. Its location cannot be changed.

The General Configuration File

The **VL_ColorCalc.cfg** configuration file is contained in the program directory. It contains

- definition of the start routine, if the software is co-installed with **VISION*lite***,
- definition of the data directory path, as defined with the software installation,
- user name appearance (see below),
- definition that users must not enter specific **Operator** names,
- definition of the main window's background color, see below.

Definition of Start Routine

If the file includes the definition of a start module *StartupModule=VISIONlite.exe,* the software shows the **Change application** function in the **File** menu that allows returning to the VISION*lite* start module.

Defining the User Name Appearance

The parameter **UserNameMask= 1-15** or empty defines the appearance of the user name in the **Operator** text box. The following options are available:

1	Domain or PC name
2	Login name
4	Full user name in brackets
8	Description

The figures can be added. The default setting (parameter empty) is equivalent to the setting *7 = 1 +2+4*. Thus the user name is given as:
Domain or PC name\login name (full user name) (if available).

Login Operator names

The **UseWindowsUserName=1** configuration option defines that the software does not allow entering an operator name. Instead always the Windows login name as defined above is applied.

Modifying the main Window's Background Color

The **BackgroundColor** parameter allows modifying the software's main window background color. If no value is given, the default Windows background color is applied. To change to a different color, enter for example

BackgroundColor = &HE8FFFF

to achieve a light yellow color.

A color is defined by its RGB value in hexadecimal notation with the prefix *&H*.

8.2 Options in the Configuration File

A number of options is defined by editing the software´s configuration file **VL_ColorCalc.ini** in the **Data** directory.

Important:
When editing the configuration file, first close the software. Otherwise the file will be overwritten, when the software is closed. Generate a backup of this file before any modifications are done.

The configuration file has the sections:

[Directories]
[Configuration]
[Spectrometer]

Each parameter in these groups has the syntax **Parameter = setting**.

Settings in the [Directories] section

This section holds the paths for the method and the results directory. Modifications are done via the **Options/Preferences** command. The modified settings are saved in the configuration file, when the software is closed.

Settings in the [Configuration] section

This section summarizes parameters for general software operation.

Parameter	Default	Options	Relevance
PageFooter=	Software Name	Text	Text entry for the report footer. Modification via the **Options/Preferences** command; automatic entry with software termination.

Parameter	Default	Options	Relevance
PrintFormat=	0	0, 1	Printout in portrait/landscape format; modifications see above
PrintFontSize=	9	8-12	Font size of report printout; modifications see above
PrintMode=	Auto	Auto/Color/ Monochrome	Print mode. See: *Print Commands* 5-5. Modification via the **Options/Preferences** command and automatic entry with software termination.
PrintMetafile=	-	Enhanced	This setting prints the graph with thin lines.
ListSeparator=	-	e.g. "Tab", ";" , <Space>	Defines the list separator character for the spectrum export as a csv file. Without a setting, the default Windows list separator is applied.
Ordplus=	-	1	This option allows to have 5 significant places instead of the default 4 places for the live display, the axis scaling and the cursor readout. With the selection "1", %T and %R data will then have 2 decimals and absorbance data 4 decimals.
SP_Ext=	-	.dx, .csv	The parameter defines that the usual spectrum storage in the .dsp format is replaced by the csv or the dx format. Make sure that the dot is included.
ExportFormat=	-	2, 16	This parameter specifies the format of the csv file. Without setting, the file has 2 header lines (Info and column heading, e.g. nm and %T). With the setting „2“ no header is included, with „16“ only the column header is included.
ExportExt=	-	.xxx	This parameter defines the file extension for the exported spectrum. Without setting, the extension .csv is applied. Make sure that the dot is included.
ExportResultsPath=	-	Folder	If a directory path is given for this parameter, results are stored automatically in tabular form as a csv file in the given directory. The filename is the name of the (first) spectrum. Storage is independent of the **Save automatically** option.
JCAMPExt=	-	.xxx, z.B. .jc	This parameter defines the file extension for the export in the JCAMP-DX format. Without setting, the extension .dx is applied. Make sure that the dot is included.
JCAMPFormat=	-	1-15	This parameter defines the number of ordinate values within a line of the data block of the JCAMP-DX spectrum file. Thus, an adaptation to the importing software is possible. Without setting, a single ordinate value per line is applied.
TextExt=	-	.xxx	This parameter defines the file extension for the result export as a text file (parameter TextResultsPath). Without setting, the extension .txt is applied. Make sure that the dot is included.
TextResultsPath=	-	Folder	If a directory path is given for this parameter, results are additionally stored automatically as a text file in the given directory. The filename is the name of the (first) spectrum and the extensions is as above. Storage is independent of the **Save automatically** option.
PDFResultsPath=	-	Folder	If a directory path is given for this parameter, the report is stored automatically as a PDF file in the given directory. The filename is the name of the (first) spectrum. Storage is independent of the **Save automatically** option.
PDF_DirSelect=	-	1	This option allows activating the **File save as** window for PDF export from the **Print preview** window.

TextResultsPath=	-	Folder	If a directory path is given for this parameter, results are additionally stored automatically as a text file in the given directory. The filename is the name of the (first) spectrum and the extensions is as above. Storage is independent of the **Save automatically** option.
NoBlank=	-	1	For service purposes it may be necessary to perform a measurement without prior baseline correction. With the setting "1", the baseline correction run is not mandatory.
AlwaysBlank=	-	1	This parameter allows to force a baseline correction before each sample or sample group. The setting "1" is saved, when the option **Measure blank** in the Sample Information window is activated. The setting is reset by deactivating the **Measure blank** option.
EditStandards=	-		Not applicable
NameIncrement=	-	0	Sample names within a series of samples (not sample list) ending with a character are automatically incremented for the next sample. To avoid this behaviour, set this parameter to "0". Thus the **Sample Name** cell of the **Sample Information** window will be empty with successive samples.
AutoIncrement=	0	0, 1	By selecting "1" for this option, this automatism is activated: If a sample list file uses incremented spectrum names (e.g. water006, water007, water008, etc.), the system checks for the presence of spectra with the same root name (e.g. water). If present, the spectrum name is automatically incremented to the first "free" spectrum name. Thus the same list file can be used repeatedly without overwriting spectra.
KeepSampleInfo=	-	1	Within a series of samples, the sample description of the previous sample is not transferred to the following sample. Apply the setting "1" for this parameter to transfer the entries. However, the entry still can be edited or extended.
DeleteSampleList=	-	1	If a sample list with the name of the active method is present, this sample list will be applied automatically. By setting this parameter to "1", the sample list is automatically deletes after all samples have been measured. Thus an external routine can provide a new sample list of the same name.
SuppressRawData=	-		Not applicable
SpectrumReadTypes=	-	*.xxx,*.yyy, etc.	This parameter defines the file extensions offered by the **Load Spectrum** command. Without a setting, the extensions *.dsp; *.asc; *.csv; *.dx are shown.
DataSetReadTypes=	-		Not applicable
Graph_NumOnlineCurves=	20	1-50	This figures defines the maximum number of spectra that are overlaid in the graph. If the number is exceeded, the first "old" spectrum is removed.
GraphYCursorRounding=	3	3,5	Number of significant decimal places for the horizontal cursor steps.
GraphAccessScan=	0	0,1	Opens the **File** menu and graph operation tools during a scan.
GraphPermanentExpandX=	1	0, 1, -1	Directs abscissa adaptation with Graph/Permanent option: 0: adaptation to new spectrum, 1: adaptation to both spectra, -1: fixed range.
SaveText=	-	0,1	With this option, the result file is stored as a pure text file with the *Save automatically* option.

TextResultsPath=	-	Folder	If a directory path is given for this parameter, results are additionally stored automatically as a text file in the given directory. The filename is the name of the (first) spectrum and the extensions is as above. Storage is independent of the **Save automatically** option.
UpdateSpectrumList=	5	time [s] or 999999	Time interval of the Spectrum list update with an offline installation; 999999 stands for never.
MultiInstance=	-	0/1/-99	This option allows multiple parallel the software starts. With "0", a second main window is possible, if opened to display an associated file (a "." must be included in the command line, e.g. a spectrum name). "-99" never allows to start a second instance of the software.
UserParameters=	-	-	Not applicable
UpdateSpectrumList=	5	1-999999	Offline mode only: The parameters [s] defines the frequency of updating the **Spectrum** list box. An entry of "999999" is equivalent to "no updating".

Settings in the [Spectrometer] section

This section summarizes parameters for specific instrument information and settings. (Not applicable for an offline operation/installation.)

Parameter	Default	Option	Relevance
Type=	acc. installation	Helios, Genesys	Group of Thermo Scientific spectrometers
Port=	acc. installation	1-32	Number of the interface, where the spectrometer is attached. Changes are possible by software functions and are stored, when the software is terminated.
ASPort=	acc. installation	1-32	Number of the interface for the autosampler. Only for software versions that control an autosampler.
TCPort=	acc. installation	1-32	Number of the interface for the temperature controller (only if attached)
TC_Name=	-	Text	Designation of Peltier Accessory (only if attached)
TC_Serialnumber=	-	Text	Serial Number of Peltier Accessory (only if attached)
TC_Firmware=	-	Text	Firmware version of Peltier Accessory (only if attached)
InitCommand1=	-	Text	Command definitions that are sent to the spectrometer in series after the communication has been established, e. g. to define certain basic instrument settings. Further command definitions up to *InitCommand99* can be added.
InitCommand2=	-	Text	
InitCommand3=	-	Text	
Cellholder=	6	3/6	GENESYS series only: Specifies the cell changer configuration (3: 3 long-path positions). Changes are possible by software functions and are stored, when the software is terminated.
BaselineMinutes=	-		Not applicable
MaxCell=	-	1-16	This parameter allows reducing the number of active cell positions to the given number. With x=1 the cell changer is driven to position 1 for each measurement. A sample list

Parameter	Default	Option	Relevance
			can be entered. For x=0 the cell changer remains on its current position.
SipperFactor=	-	Number	Evolution 300 only: Conversion factor of sip-volume to sip-time. The entry is generated by the software's sipper calibration function and is sent to the instrument.
SipVolume=	-	Number	Only for internal use
SipperNoReturn=	0		Not applicable
Remote_2_Only=	0		No applicable
StandbyTime=	-	Number	The parameter sets the time for automatic source switch-off after a measurement.
IgnoreDSR=	-	0/1	With this option active, the software will not observe the Data Set Ready line (DSR) of the serial interface. This might help with an RS-232 communication problem.
PMTGain=	-		Not applicable
AccInitMessage=	-	text	Meassage to be displayed before an accessory initialization.
EV2_OVC=	-		Not applicable

8.3 Options in the Software Start Line

Some options for software configuration can be defined in the software startup:

1. Right-click on the program icon or the program entry in the Windows **Start** menu and select **Properties** to open the **Properties** window.
2. Display the **Link** tab.
3. Add the required option to the **Target** entry box.

Information in the Title Bar

To place an additional information text in the title bar of the main window, e.g. the instrument identification number, this information is added to the program start line in square brackets.
Example: c:\Program Files\VL_ColorCalc\VL_ColorCalc.exe [Laboratory 1]

Software Start with Predefined Method

A call of the software (either by another program or with the desktop icon) can be extended by adding the name of a method, separated by the "/" character.
Example: The call c:\Program Files\VL_ColorCalc\VL_ColorCalc.exe /test1.mol will start the software with the method test1 and will proceed to the sample information entry.

Tip: *The desktop may include several software icons with different definitions.*

If the software is configured to the offline mode, also a spectrum file may be transferred.

The following, additional options are available for routine operation:

/edit Opens an option to modify definitions of the parameter definition file within the

	software; see section *Calculations Window* 5-21. Set by starting the software with a double click on *VL_ColorCalc-Edit.bat* in the software's program directory.
/export	Generates a result data export file in CSV format, if at least one result has been calculated.
/print	Prints the report automatically, if at least one sample has been measured.
/ terminate	The software is closed automatically after finishing the sample series.
/preview	Opens the preview window, if at least one sample has been measured.
/pdf	Stores the report as a PDF file, if at least one sample has been measured.
/text	Stores the results as a text file, if at least one sample has been measured.

Example: The call c:\Program Files\VL_ColorCalc\VL_ColorCalc.exe /test1.mol /print / terminate will start the method test1, configure the spectrophotometer, and open the sample information window. After the sample series, the report is printed and the software is closed.

Deactivating the Obligatory Baseline Correction

Usually a background correction run must be performed after the software has been started or after extension of the wavelength range. This is good laboratory practice and it is required for accurate and reliable results. When measurements should become possible without a prior background correction run, e.g. to check the instrument, the start line can be extended by the **/ noblank** parameter.

Number of Cell Changer Positions

When a cell changer is detected with the instrument, the sample information window offers as many sample lines as positions are available with the cell changer. It is possible to reduce the number of used cell positions with the **/maxcell**<number> parameter. <number> is the number of active cell changer positions.
Example: c:\Program Files\VL_ColorCalc\VL_ColorCalc.exe /MaxCell2 will reduce the number of available cell positions to 2.

- With x=1 the cell changer is driven to position 1 for each measurement. A sample list can be entered.
- For x=0 the cell changer remains on its current position.

8.4 Reflectance Measurements

In order to measure reflectance data the spectrometer must be equipped with a dedicated reflectance accessory like an integrating sphere or a specular reflectance accessory. In this case the **Measurement mode** is selected as **%R**. (See: *Spectrophotometer Group* 5-17) The software will still read **%T** data from the spectrometer, but will correct the readings for the white standard and the dark value online. The respective spectra for these corrections have to be present as stored spectrum files.

For specific applications in reflectance spectroscopy the additional **f(R)** mode (recalculation of reflectance data according to the Kubelka-Munk function) and the **%Ra** mode (square root of reflectance data for absolute reflectance measurements with a V-W accessory) are available. A reflectance correction is not applied for the **%Ra** mode.

Tip: *Measurement with an absolute reflectance accessory like V-N accessories do not require a reflectance correction and therefore must be executed with the* ***%R*** *ordinate mode with a reflectance correction "**Null**", see below.*

The Principle of the White Standard Correction

The white standard correction is necessary since the baseline run assumes that the white standard reflects 100 % of the incident beam. However, in practice a white standard typically has an absolute reflectance value in the range of 90 – 99 %R. Therefore all untreated readings are too high. This discrepancy is taken into account by simply multiplying the raw data by the absolute reflectance data of the white standard. The spectrum used for this calculation must contain the white standard reflectance data for the whole wavelength range covered by the sample spectrum. The data typically are supplied by the distributor of the standard.

The Principle of the Dark Correction

The necessity for the dark correction is based on the fact that due to the construction of the spectrometer a small portion of the measurement light will be detected without striking the sample. It can also become necessary, when a strongly transmitting sample is covered by a light trap that has a small residual reflectance. If not taken into account in these case, weakly reflecting samples samples will show slightly too high readings.

The dark correction values can be identified by measuring the reflectance spectrum of an empty sample position after baseline correction. The sample position should be covered e.g. by a black cloth acting as a light trap and as a protection from room light. With proper instrument alignment, dark correction readings should not be higher than a few %R.

When the measurement uses a light trap, the applied trap should be measured.

Important: The measured dark correction spectrum should be measured against the reflectance standard that is also employed for sample measurements. However this measurement must remain uncorrected (reflectance correction "Null", see below), because these data are subtracted from the instrument's raw data.

Tip: *Measuring the dark correction data should be done with an optimal signal-to-noise ratio, e. g. with reference beam attenuation, high integration time and high spectral bandpass. It may also be considered to carefully smooth the spectrum after measurement.*

Significance of White and Dark Correction

White and dark correction procedures are especially important if absolute sample reflectance values must be generated, for example for color evaluations or for quality control of AR coatings, especially when very high or very low reflecting samples are to be examined.

The described corrections are irrelevant, if only qualitative measurements are performed, e.g. to compare two samples or to determine absorbance band positions.

Options for Reflectance Measurements

The software offers several default data sets for reflectance correction in the **Advanced Parameters** window of the **Spectrophotometer** parameter group. See: *Advanced Parameters window* 5-19

Table: Default reflectance corrections

	Wavelength [nm]		
Type	**Range**	**Interval**	**Comments**
Null	200–3000	10	Value of 100 %R for the white correction and a value of 0 %R for the dark correction. Obviously this set does not modify the raw data.
BK7	200-2500	2	Front surface reflectance curve of a standard BK 7 glass for the white correction and 0.0 %R for the dark correction.
Spectralon	200–2500	5	Typical reflectance curve of Spectralon® for the white correction and 0.2 %R for the dark correction.
Barium sulfate	380-780	1	Typical reflectance curve of $BaSO_4$ white reflective material for the white correction and 0.2 %R for the dark correction.
Al mirror	250-2500	10	Typical reflectance curve of a coated front surface aluminum mirror for the white correction and 0.2 % R for the dark correction.

For that the software applies system files for white and dark correction. The files are csv files (comma separated values) as created by MS Excel® resident in the software's program data directory. See: *Data Formats and Import/Export* 9-1

- White correction files <*Name*>*.R100.csv* (e.g. <Name> = *Null*)
- Dark correction files <*Name*>*.R0.csv*

A check of the correction files is possible by loading the spectra from the **Data** directory. See *Preferences* 5-12.

Preparations for Reflectance Measurement

If you want to use the white and dark correction of reflectance measurements, you should adapt

these files according to the specific spectrophotometer and white standard in use or create new files following the scheme. The data interval is deliberate, because the software interpolates the data as required. Use the Windows editor/notepad or a spreadsheet program to edit the data in the files.

- Enter the absolute reflectance data of your white standard (as received from the supplier) and store the table as *<Name>.R100.csv* file in the Data directory.

- Enter the dark value readings as measured with an empty reflectance sample position and store the table as *<Name>.R0.csv* file in the Data directory. You also may use the measured spectrum directly by storing it as a *<Name>.R0.csv* file with the appropriate name to the Data directory.

After software restart, the additional *<Name>* identifier will appear in the **Reflectance Correction** selection box (**Advanced Parameters** window).

***Note**: The files used for white and dark correction must cover the total wavelength range of the sample spectra. If not, it is not possible to record the data in **%R** mode. If the data interval is not identical, the correction values are correspondingly interpolated.*

***Note:** For every corrected spectrum, the software registers whether and with which data files the reflectance correction was performed. You can inspect this information in the **Spectrum** information window under **Audit trail**. If you create your own **<Name>.R0** and **<Name>.R100** files, you should include a detailed commentary in the spectrum description so that the correction is traceable.*

8.5 Adapting the Report Header

The report includes an alphanumeric header that summarises various information about measurement parameters and instrument settings. An option allows adding additional user-specific information as a report header lead text and/or a report header trailer. This option is helpful, e.g. to generally implement specific company or lab information or to add further lines with system-specific information.

This is accomplished with the use of two temporary text files with dedicated filenames. The files must be present in the results directory.

The text files are detected by these filenames:

MO_METH_HEADER1.tmp	This text is added as a header above the default report header.
MO_METH_HEADER2.tmp	This text is added as a trailer below the default report header.

***Tip**: Please note that the text information is not added to the results section of the program window, but only to the report before printing or with **Print Preview**.*

The text files should be generated by the Windows Editor/Notepad and do not allow any formatting. The files are automatically deleted, when starting a new measurement series, as far as they are not protected by a read-only flag. Thus a new report header file can be inserted for any new measurement.

If however, the files are write-protected, they will be applied to all generated reports. Thus the files will still be available for further offline report generation and for further measurements.

Tip: It is also possible to integrate a graphical logo to the report; see section *Report*

Configuration 8-35.

8.6 Protected Methods

When the method file has the read-only attribute, the method cannot be modified by the user or be overwritten by the **Save Method** command.

To establish the read-only status for a method:

1. Open the current method directory with the Windows Explorer. See: *Preferences* 5-12
2. Right click on the requested method file and open the **Properties** window.
3. Activate the **Read-Only** attribute. See: *Preferences* 5-12

When a write-protected method is selected, the parameters are shown as usual, but all parameters and buttons are blocked. This is depicted by grey headings in the parameter area and a red hint **write protected** above the **Method** list box. See: *Parameter area* 5-15

An error message is given, when the user tries to store a method with this filename.

Note: *It is recommended to protect frequently used methods with this option. The option is designed to prevent an accidental modification of methods. However, to protect the software against deliberate manipulation of the methods, further operator and security settings must be defined by the system administrator.*

8.7 Data Handling Templates

Templates with scripting functions are applied to generate menu functions in the **Measure** menu and in the **Data Handling** menu. See also *Measure Menu* 5-7 and *Data Handling Menu* 5-8.

The templates are identified by their name ***, identifier and the file extension .rpx. The name gives the name of the function, whereas the identifier (SC, etc.) defines the position of the function:

***.SC.rpx or ***.DH.rpx	**Data Handling** menu
***.MS.rpx or ***.MA.rpx	**Measure** menu

When the software is installed together with VISION*lite*, the ***.DH.rpx and ***.MA.rpx templates appear in all applications.

Further templates files with scripting functions are installed to the software's \Tools directory. To utilize them, copy the respective file to the software's Data directory and restart the software. See also the *Read_me.txt* file within this directory.

Tip: *The functions can be renamed by modifying the template file name ***. The functions can be removed by deleting the corresponding template.*

The following commands can be additionally made available in the **Data Handling** menu:

- **%RtoFR** The function converts all %R spectra that are displayed in the graph to spectra with the Kubelka-Munk ordinate F(R). This ordinate typically is applied for quantitative reflectance measurements.

- **Abscissa Shift** — Shifts the start and end wavelength of the spectrum with the entered value. Thus it is possible to correct for a wavelength scale error or simulate a wavelength shift by some sample treatment, e.g. modified layer thickness of a thin film system. Otherwise the spectrum stays unmodified and is not stored to disk.
- **Absorption Coefficient** — The function allows calculating the molar and the specific absorption coefficient from the spectrum at a selected wavelength. Sample concentration and cell thickness are queried.
- **Attenuation 10%, Attenuation 1% Attenuation 0.1%** — The functions perform an offline correction of a sample spectrum after an attenuated measurement. Each function divides the displayed spectrum (%T or %R) by the respective attenuator spectrum and multiplies by 100. The attenuator spectrum must have the name *RearAttenuator??.dsp*, where ?? = 10, 1 or 0.1 stands for a 10%, 1% or 0.1 % attenuator. Typically this is the measured spectrum of an attenuator sieve.
  The spectra must have the ordinate mode *%T* and must be stored in the Data directory. Synthetic test spectra with the designated %T values are available in the CD's *tools* directory.
- **Average incremented spectra** — Calculates the average of those spectra in the graph that have identical measurement parameters and that share a common body name with a numerical incrementation. The incremental figures can be positioned at any place in the name; they must start with 1 and may go up to 9 without a missing figure. Multiple groups of incremented spectra are treated. The results file has the body filename and it has an appropriate description. The source spectra are deleted from the graph.
- **Change Ordinate** — The routine allows changing the ordinate of an absorbance spectrum (ordinate A) i the graph.The selection offers the equivalent modes **o.d.** (optical density), **Abs** und **AU** (absorbance unit) as well as **dB** (A * 10) and **mA** (A * 1000). The modified spectrum replaces the original one in the graph, but t is not stored automatically.
- **Convert Abscissa (~)** — The routine starts with a spectrum with the ordinate mode **nm** that is typical for UV/Vis(/NIR) spectra. Data are recalculated to an energy proportional ordinate mode. The selection offers **cm-1** (wavenumber), **eV** (electron volt) and **THz** (terahertz). The data interval of the target spectrum is selected such that it is similar to the original data interval in the middle of the spectrum range. Linear interpolation is applied to generate new ordinate values at the data points. The modified spectrum replaces the original one in the graph, but t is not stored automatically.
  The second routine (attached ~) additionally in the graph turns the orientation of the abscissa so that the spectrum is shown with decreasing ordinate values as typical in IR spectroscopy.
- **Double Grid** — This function divides the grid lines distance to halves and adds grid lines to the diagram for both axes.
  However with this process, the grid scaling is fixed so that it does not adapt to scale changes. This is re-opened with a new measurement.
- **Norm1** — The function transform the %T or %R spectra of the diagram to T or R immediately. The data are divided by 100 and the ordinate mode is replaced accordingly.
- **Norm100** — The function transforms the T or R spectra of the diagram to %T and %R spectra. Thus it reverses the action of the above *Norm1* function.
- **Ordinate Average** — Calculates the mean ordinate value over a specified wavelength range. The result value shown in the results area.

- **Set Line** Inserts a horizontal line in the spectrum graphics at the defined ordinate value. The line is handled as an additional spectrum.
- **Set Operator Name** Allows selecting an operator name independently from a measurement.
- **Smooth_MA** Applies a moving average (MA) smooth calculation to the spectra displayed. Otherwise as described for the normal **Smooth**.

With these routines, the generated result spectra are not stored automatically. Use the **Spectrum** information window to store the result spectra individually. See: *Spectrum information* 5-30 window.

There are some templates for specific evaluations. Copy the respective template from \Tools directory to the Data directory of the software.

- **Read DTA file and start calculation** Reloads the parameter definition file - after a modification - and starts an evaluation of the displayed spectra with the active method based on the new parameter definitions. The software must not be re-started. Thus a fast optimization of result presentation becomes possible.

Further templates <*Name*>*.DH.rpx* or <*Name*>*.MS.rpx* with utility functions can be activated as described above. Due to the *MS* tag, the functions **Read DTA file ...** and **InstCommand** are allocated in the **Measure** menu.

- **Comment Results** The function allows inserting a text to the result area. The option can be used to add a comment to the measurement result.
- **Copy result table to clipboard** Copies the results in the results area to the clipboard in a tabular form (csv-format). The tab character is applied as the separator character so that the information can be readily pasted to a spreadsheet program.
- **Copy graph to clipboard** Copies the graph area to the clipboard. This information can be readily pasted to a publishing or other program.
- **InstCommand** Instrument commands can be typed and sent directly to the instrument. The instrument response is shown. This option should be used by experienced service personnel only - refer to the instrument documentation for the correct instrument command syntax.

If you should require further calculation or utility functions, you can generate these with the optional **Reporter-SPX** software. Alternatively contact ***ascanis*** directly.

8.8 Linking of External Routines

The software allows automatically executing external executables at defined points during the measurement sequence. These "subtasks" are activated at the opening of the sample information window or the start/end of the measurement. The link point is defined through its name. The executables receive specific parameters like the sample or method name from the main software.

A subtask can be an exe-file, a batch files or a Reporter-SPX templates. If it exists in the program directory, it will be started for each measurement. However, the routine can be

programmed so that it responds only to a specific sample or method.

An example can be applied to present information to the user at the start of the measurement. Copy the files *MO_RunStart.exe* from the /tools directory on the CD to the software's program directory. Then create a text file (extension .txt) or a PDF-file (a PDF reader must be installed) with a file name that is equivalent to the method file to be executed. Copy the file to the methods directory. The routine is started with each measurement: If it detects a text or file with the name of the active method, this file will be reproduced in a separate window. Otherwise the routine remains inactive. Thus, each method can be backed up by an information text.

When you copy the *MO_RunEnd.exe* example as above, generally after a successful termination of a measurement, a sound (Windows default beep) will be output three times to inform the user.

The subtask option can be employed for numerous further purposes: It may allow controlling external devices like a temperature readout during the measurement process or integrating application-specific sample data or result handling, like importing these from a LIMS system.

The following subtasks can be applied:

Name of subtask	**Startup with ...**
MO_APPSTART1	Start of application before communication to instrument
MO_APPSTART2	Start of application after start of communication to instrument
MO_SAMPINFOSTART	Opening of the Sample information window
MO_SAMPINFOEND	Closing of the Sample information window
MO_RUNSTART	Start of a measurement series
MO_ACCSTART1	Start of an accessory control
MO_ACCSTART2	End of an accessory control before measurement
MO_ACCEND	End of an accessory control after measurement
MO_SAMPLESTART	Start of sample measurement
MO_SAMPLEEND	End of sample measurement
MO_RUNEND	Termination of a measurement series
MO_RUNERROR	Error during data transfer from instrument
MO_APPTERMINATE	Closing the application

You are welcome to request further information or support for this option.

8.9 RLS-Export

The template *RLS_Export.SC.rpx* allows exporting a spectrum file as a text file. The text file format can be configured. The file is exported to the *Results* directory and it has the file extension *.rls*.

An extended template *RLS_Export_VarInt.SC.rpx* additionally allows selecting the data interval of the spectrum.

The template is available in the *\tools* folder of the software CD. To utilize it, copy the file and the layout file *RLS_Export.txt* to the software's Data directory and restart the software. The function is then present in the **Data Handling** menu:

The exported text file typically has a header and a data section. Details of both sections are configured by the *RLS_Export.txt* layout file. The layout file mirrors the desired output. The various figures and information taken from the spectrum are represented by $variables (name with preceded $-character).

The following $variables apply:

Variable	Placeholder
Spectrum name	$SI
Description	$SC
No. of data points	$NP
Data interval	$AD
Upper (start) wavelength	$AH
Lower (end) wavelength	$AL
Ordinate unit	$OR
Instrument name	$IN
Method name	$M
Path name	$PT
Double polarizer position	$PL

$Variables for Text Input

The following placeholders are used to generate the data table:

Variable	Placeholder
Abscissa value	$W1
Ordinate value	$V1
Repetition character	$R

The $variables $W1 and $V1 represent abscissa and ordinate values of the spectrum. With an

repetition character at the end of the data table line, the line will be repeated up to the last data point.

$Variables for Text Input

A query for additional user entered information can be implemented via the $TX variable. The variable opens a window for text input. The text is placed at the variable's position. An entry length and a user query text can be added in square brackets.
Example: $TX[20][Name of coating]

Example

A *RLS_Export.txt* layout file can have this appearance:

```
Spectrum:      $SI
Comment:       $SC
No. of data points:      $NP
Data interval:      $AD
Ordinate units:      $OR
Instrument Name:       $IN
Methode Name:   $M  $PT C:\Temp
Double Polarizer:   $PL
Coating name:   $TX[20][Coating name]
Polarization:   $TX[4][Polarization]
Angle of incidence:   $TX[4][Angle of incidence]
Sample compartment:   $TX[20][Sample compartment]

Abscissa   Ordinate
--------------------------------
$W1          $V1$R
```

8.10 Adapting the Evaluation Parameters

The list of all possible calculation parameters is given in the parameter definition file **VL_ColorCalc.dta** in the Data directory. The file is a text file. It can be modified with options of the **Calculations** window; see *Calculations window* 5-21.

The editing option is conveniently made available by starting the software with a double click on *VL_ColorCalc-Edit.bat* that is found in the software's program directory.

Alternatively, use the Windows Editor/Notepad or import it to Microsoft Office Excel for direct modifications of the definition file.

Important:
Generate a backup, before editing the parameter definition file.

Each line of this file represents a calculation parameter. A semicolon as the first character recognizes information lines, which do not define a parameter. Setting a semicolon also allows deactivating parameter lines, which are currently not to be used.

The file can be extended, rearranged, or abbreviated to your specific laboratory requirements. Parameter definitions can be modified. Also, new parameters can be added based on the given syntax. See section *Syntax of Parameter Definitions* 8-18.

The parameter definitions are numbered. The numbers organize the parameters to groups with a tree structure. Additional parameters should be inserted to free number positions. The numbering order must be maintained.

It is also possible to suppress the result output of a selected parameter line by format definition, e.g. if the result is required only for further calculations. See: *Syntax of Parameter Definitions, Section 4* 8-18.

Most parameters refer to a given energy or response data files <name>**.dat** that are encoded. New parameters may use existing **.dat** files. Alternatively also new files can be defined that need not be encoded. See section *Format of Data Sets.* 8-22

Note: *The modified parameter definition file will become active after the software has been restarted, but see below.*

Tip: *The /tools directory of the software CD includes a tool for an immediate activation of the parameter definition file: Copy the file "Read DTA file and start calculation.MS.rpx" to the Data directory and restart the software. Open the VL_ColorCalc.dta file with the notepad/editor, modify the file and save it. Then load a test spectrum and click the new "Read DTA...." command of the Measure menu. You can immediately view the results of the required calculations based on the modified parameter definition file.*

8.10.1 Syntax of Parameter Definitions

Each parameter definition line contains at least four sections (except comment lines), separated by the tabulator character (represented by “Tab” in the following):
Parameter No. (nnn_mmm_ooo) "Tab" Calculation type "Tab" Short description "Tab" Output format "Tab" Long description "Tab" Ordinate mode(s)

*Example: Example:100_001_001"Tab"F:SA.dat*VL.dat"Tab"tVIS (EN 166/169/170)"Tab" : [1.3]"Tab"Luminous Transmittance (DIN EN 166/169/170)"Tab"%T*

The ordinate mode(s) entry is optional. Additionally, sample information text can be added, see below in section 4.

The above example parameter line will appear in the list of parameters of the Calculations window as

tVIS (EN 166/169/170).

When selected, the information below the **Calculations** window will show: (see: *Calculations Window* 5-21)

Luminous Transmittance (DIN EN 166/169/170)

The output line within the report will be:

Luminous Transmittance (DIN EN 166/169/170): n.mmm %
(n.mmm: Result value with 1 digit before and 3 digits after the comma)

The example calculation is performed only for %T spectra. It is suppressed, when the spectrum has a different ordinate mode, see below.

Section 1 Parameter Number

The parameter number is unique to each calculation parameter and it describes its position within the sections. The number has the format *nnn_mmm_ooo* that allows setting up a tree-structure: The first 3 figures *nnn* designate the main section; the second group of 3 figures *mmm* designates the position of the parameter or a sub-section. Figures *ooo* designate the parameter

within a sub-section.

Free number positions can be applied for further parameters and numbers can be modified. However, the order of numbering should be maintained. Otherwise the parameter are disordered in the **Calculations** list and an error message is shown with the software start:
System error during run: Listing key is ambiguous.

Parameter definitions lines with a leading semicolon are set inactive (hidden).

Section 2 Calculation Type

The calculation type is defined by the leading character with a double point. This character can be detailed by another character defining a calculation subtype. This definition is followed by the employed data set(s). The following table shows the characters used.

Table: Characters for Selection of the Calculation Type

Character	Calculation type
C:	Color values, subtypes: X-, Y-, x-, y-, z-, L-, C-, h-, D-, P-, E-, J-, Z-, W-, G-, S-, special characters for whiteness and yellowness index and tint
S:	Special calculations, subtypes: A-, B-, 1-, 2-
E:	Mathematical calculations with spectral values
K:	Comment lines, headings

Note: *Not all calculation types may be available for this software version.*

Data sets are data files with the filename extension **.dat** residing in the Data directory. The data sets contain the required tabular data for the calculations, like the D65 source spectrum.

Additional Identifiers for the Definition of Calculations

For some evaluations like C:D and M with spectra, referenced spectra are appended to the calculation definition with a * (asterix).
*Example: C:D-D6510grd.dat*ref1.dsp"Tab"Color difference (D65) to spectrum ref1"Tab"….*

Section 3 Short Description

The short description is a text characterizing the calculation within the **Calculations** selection box. This text does not appear in a report. See: *Calculations Window* 5-21

Note: *Generally the user may modify these texts. However, the short description text for DAB/EP colors, for APHA, Gardner and iodine color values must remain unmodified because otherwise the required calibration data cannot be loaded.*

Section 4 Output Format

This section defines the appearance of the numerical results. It basically may comprise a prefix, the actual number format, a suffix and the mask character string *!§* (exclamation mark and paragraph).

Note: *Defining the output format can be omitted; however the tab characters must remain.*

Any alphanumerical expression before the number format will be output preceding the figure(s). This can be used to add spaces for having several output figures in line or to replace " :" by other characters.

The number format can be specified: Define the number of digits before and after the decimal separated by a point in square brackets: For example the expression [4.2] will define to print 4 numerical places before and 2 places after the decimal point.

After the number format specification, a suffix can be added to present the unit of the figure. Any character except the comma can be applied. If **%** is selected with the convolution type calculations, the result of the calculation is multiplied by 100.

It is possible to completely mask the output of the selected parameter, e.g. to apply it solely for a further calculation or decision. This is done by inserting the mask character string !§ at any position within the output format.

Multiple Figure Output

Some evaluations like C: or S:1- output more than one figure in the result line, e.g. Lab-color values. Here, each figure can have its own description and numerical format.
Example: Color difference can be presented by ..."Tab"DE: [3.1]; DL: [3.1]; [0.0][0.0] DC: [3.1]; DH: [3.1]"Tab"...

The format **[0.0]** will prevent the respective figure to be output. Thus it is possible to restrict the output to a specific result.

Introducing a pipe symbol (|) after a numerical format definition generates a line feed at this point within the output.
Example: The output uses a new line after DE: ..."Tab"DE: [3.1]|DL: [3.1]; [0.0][0.0] DC: [3.1]; DH: [3.1]"Tab"...

Integration of Calculations and Decisions

It is possible to integrate calculations, decisions and decisions on calculated values into the output.
Example: the Gardner color value output ..."Tab"{abs([0.0][1.1]-0.5) <= 0.5[Sample within Gardner scale][Sample out of Gardner scale]}<Tab>...

The expression has to be put into curly braces: "{" and "}". It uses the syntax as described for arithmetical expressions. See section *Calculation Expressions* 8-23. The above example checks, whether the decimal section of the result is less than 1.

When an evaluation outputs several figures, each result value can receive its specific calculation.

It is possible to conditionally mask the output by using the mask character string described above.
Example ..."Tab"{[1.3] <= 0.5[Sample OK][!§]}"Tab"...

Integration of Classifications

The output of results can also be changed to a classification of the results. This allows classifying samples according to their numerical results, e.g. to output the UV protection level of a sample according to a table of limit values. See section *Sample Classification* 8-33 for further details.

Note: *You cannot combine an output of a figure with a decision or classification. If both is required this has to be done in two separate lines.*

Section 5 Long Description

The long description text of the parameter is shown in the **Calculations** window below the list box, when the parameter is selected and in the report. See: *Calculations Window* 5-21

For for the EP color examination, the long text must consist of 2 sections separated by a double point. When the result is true, the first section is output. If it is false the second section is output.

An optional sample information can be appended. To implement it, a text is added to the parameter definition separated by a “|” (pipe) character. Texts for further spectra of a series of samples can be added likewise separated by a “|”.
Example: F:MW8100.dat"Tab"AV 800-1000 nm"Tab" : "Tab"Average 800-1000nm|Sample1|Sample2|Sample3

During the measurement process, the sample information is automatically inserted to the **Description** entry field of the **Sample Information** window. It can however be further modified by the user. For example, this option allows giving special measurement hints to the user.

The **Haze** parameter applies this option to identify the specific measurement procedure for the sample.

Note: *If selected evaluation parameters hold different sample information, the last information is applied.*

Note: *This option is not applicable, if a sample list is used. See Sample List* 6-5.

Format of Comment Parameter Lines

The comment parameter line is used to organize the list of parameters. It is an abbreviated parameter line with the calculation type character K: and a long and a short text:

nnn_mmm_ooo"Tab"K:abc"Tab""Tab"abcde

As with the standard calculations parameters, the short text **abc** is shown in the list of calculation parameters. The long text **abcde** with additional information is shown in the **Calculations** window below the list box and in the report.

The comment parameter lines function as section headers, but can also be selected for integration into the report to generate a subheading. A preceding blank line can be selected to separate the text block. The line with the comment long text and the optional blank line are positioned in the report at their positions in the list of calculation parameters. By extending the parameter definition file, further blank lines can be inserted at the required positions.

In a comment line, also the n-th spectrum name can be inserted as **ResultTable(n,1)** and the n-th spectrum description as **ResultTable(n,2).** See also section *Calculation Expressions* 8-23.

8.10.2 Format of Data Sets

Most calculation parameters require energy and/or response data, e.g. solar radiation data. These data files have the filename extension **.dat**. The files are contained in the Data directory and they are encoded to prevent accidental modification. The data files for min/max data sets and the single wavelength output are not encoded and have the file extension **.txt**. This is to allow user modifications.

It is possible to add additional data sets for user-defined calculations. The files are simple text files with a filename extension other than **.dat** (e.g. **.txt**). The files contain tabular data with a leading text line to describe the file. The table has the wavelength in the first column and the respective data in the second column(s). The decimal character must be a point; the column separator may by a comma, space, semicolon or tab. It is not required that the wavelength interval is uniform.
Example

Standard sun µW/(cm² × nm)	
290	0.000309
292	0.00285
294	0.0292
296	0.128
298	0.337
and so on	

8.10.3 Color and Color Difference Calculations

As described in the section *Colorimetric Evaluations* 7-5 *and Color Difference* 7-8, various color values can be generated from a spectrum. The calculations refer to a set of observer data (2 or 10 deg) and an illuminant (A, C, D65). These data are given in a dat-file (See section *Format of Data Sets* 8-22) for either the default wavelength range of 400 - 700 nm or the extended wavelength range of 380 - 780 nm. Filenames are
illuminantgrx.dat, resp. *illuminantgrxe.dat* (extended range)

An example of a color calculation definition accordingly can be:
C:X-a10grde.dat for the output XYZ values with 2 deg observer and illuminant A in extended range

Whereas the character C stands for color calculations, the second character stands for the subtype of calculations:

X-	Output of XYZ Tristimulus values and optionally X0, Y0, Z0
Y-	Output of x, y color coordinates and Y luminance value
L-	Output of L, a, b, C, h and optionally S (=C/L)

Output of a reduced set of values or single values can be achieved by blocking the unwanted results with the [0.0] number format.

Applying user-defined Illuminant and Observer Data

All color calculations are defined with an observer and an illuminant file. Additional or modified

parameter definitions can also be setup with user-defined illuminant and observer data. As an example, the files *IllumD65.txt* and *CIE1964_10.txt* are installed with the software. These files are used in a hidden parameter definition line of the parameter definition file:
*;160_701_001<Tab>C:L-CIE1964_10.txt*IllumD65.txt<Tab>.....*

This calculation is not referenced in the standard **Calculations** list, but it can be activated by removing the leading ";". With this principle, calculations with user-defined illuminants and observers can be introduced. The files are simple text files. However, spectral range and data interval of the illuminant and the observer file must match strictly.

Color Difference Definitions

As with other parameters, each line on the parameter definition file **VL_ColorCalc.dta** represents a calculation parameter, which is presented in the **Calculations** list.

The predefined examples use the illuminant/observer D65/10 and as a reference either
- the filename of the reference spectrum *max1.dsp*
- a set of Lab* values *L=10,a=0.5,b=0.5*
- or the tristimulus values *X=10 Y=10 Z=10 X0=94.7178 Y0=100 Z0=107.1163 (CIELab color difference only)*

The given X0, Y0 and Z0 values are the tristimulus values for the absolute white with the selected illuminant/observer. These can be generated with the Tristimulus values calculation. See *Colorimetric Evaluations* 7-5.

These settings are only used as example; the definition is adapted by the user: Another reference spectrum filename or a Lab* reference set can be entered and further definition lines can be added, see *Adapting the Evaluation Parameters* 8-17.

The reference spectrum is expected to reside in the results directory. This could be a spectrum just recorded from a reference. If it is not found there, it is searched in the program data directory. This could be a general reference. However, the spectrum in the results directory has priority.

The parameter line also allows defining, which illuminant/observer is used, which of the 6 difference values are output and which numbers of decimals are to be used. For the CMC color difference, the weighting can be varied.

8.10.4 Calculation Expressions

Besides using the predefined calculation parameters the software also allows defining individual calculations with spectral data and results.

Arithmetic expressions are defined in the parameter definition file. The type of evaluation is characterized by the *E:* calculation type, followed by a calculation expression; e.g. *E:YVal(500)* *(ordinate value at 500)*

The full parameter definition line could be: (see also *Syntax of Parameter Definitions* 8-18) 8-18

100_001_001"Tab"E:YVal(500)"Tab"Ordinate 500 nm"Tab": [3.3] "Tab"Ordinate value at 500 nm

There are more examples below.

The numerical result of the mathematical expression or the true/false text of the logical

expression is output together with the defined parameter designation and format.

Note: *Also, arithmetic expressions can be integrated into a calculation parameter line, see: Syntax of Parameter Definitions* 8-18

Important: With the **Thickness Correction** activated, calculation expressions refer to the corrected spectrum. Access to the original spectrum must be referenced with $1 suffix, see below. Also see: *Thickness Correction* 7-3

An arithmetic expression (formula) consists of figures, memory variables, calculation or comparison operators and spectral or general functions. If there is a syntax error or a mathematically incorrect operation, an appropriate error message is presented.

Using Arithmetic Expressions

Figures

Figures can be integers, decimal figures or figures in scientific notation. *Example: 1.23e-2 for 0.0123*

Note: *Numbers must be expressed with the decimal point.*

Additionally, **ra** variables as placeholders for numerical input from an *Ask* query and m-variables from previous numerical calculations (see sections *Ask Function* and *Memory Variables* below) can be contained.

Calculation Operators

The standard calculation symbols +, -, *, / are applicable. Additionally „!“ (factorial) and „^“ (exponential) are possible. The formula can be structured by any number of bracket levels „( )“.

Logical Operators/Decisions

The following logical comparison operators are available:

=	equal
<>	unequal
>	larger
<	smaller
>=	larger or equal
<=	smaller or equal

Comparison results are basically output as either *true* or *false* as a word. Additional texts for *true* and *false* decisions can be appended in square brackets to the formula. If available, the first text is output for the decision to be *true* and the second text is output for *false*.

Example

E:1 > 2"Tab"Decision example1"Tab""Tab"Decision result

The result of the decision is: **false**.

E:abs(94-100) <= 5 [Result in tolerance][Result out of tolerance] "Tab"Decision example2

"Tab": "Tab" Decision example 2
This will be presented as: **Result out of tolerance**

The conditional result text output may also contain figures via the *Spectrum(Parameter*) variable (see below) or numerical values from memory variables (see below). For numerical values a format may be attached to the expression as *[n.m]*.

General Calculation Functions

Trigonometric and logarithmic functions are available for use within the formula.

Table: Trigonometric and logarithmic functions

Operator	Funktion
rad()	Transformation of angle measures from degree to radian
deg()	Transformation of angle measures from radian to degree
cos()	Cosine 1)
acs()	Arc Cosine 1)
sin()	Sinus 1)
asn()	Arc Sinus 1)
tan()	Tangent 1)
atn()	Arc tangent 1)
sqr()	Square root
log()	Logarithm (decadic)
lne()	Natural logarithm
exp()	e-function
abs()	Absolute value
rnd()	Rounding to integer (note: r n d)
rnd(|n)	Rounding to n-figures after the decimal (note: r n d)
sum(n;m;o…)	Sum of the figures in parentheses 2)
min(n;m;o…)	Minimum of the figures in parentheses 2)
max(n;m;o…)	Maximum of the figures in parentheses 2)
ave(n;m;o…)	Average of the figures in parentheses 2)
sdv(n;m;o…)	Estimate of Standard Deviation of the figures in parentheses 2)
vcf(n;m;o…)	Variation Coefficient of the figures in parentheses 2)
sgn()	Leading sign of a figure (as -1, 0, +1)
fix()	Figure without decimals (e.g. fix(2,56=2))
mod(n|m)	Remainder of a division (e.g. mod(7|5)=2)
ddi(d1|d2)	Difference of the date/time values d1 and d2 in days
ddi(d1|d2|p)	Difference of the date/time values d1 and d2, expressed as p: yyyy / m / d / m / s (year, month, etc.)
iwn()	Is whole number? (0 / 1)
iev()	Is even? (0 / 1)

Operator	Funktion
iod()	Is odd? (0 / 1)
ihx()	Is Hex? (0 / 1)
ieq(<1>|<2>)	Is equal: check for equality of floating point numbers 1 and 2 (0 / 1)
iir(<1>|<l>|<h>)	Is in range: check for figure 1 within l and h (0 / 1)

1) For the trigonometric function the angle has to be given in radian measure.
2) The separator of figures can be ";" or "|"

The argument of a function is appended in brackets.

Example

log(50+50)	The result of the calculation is 2.
rnd(sqr(5)|2)	The result of the calculation is 2.24.

Tip: *As well, least-squares regression calculations can be integrated; contact* ***ascanis*** *for further information.*

Spectral Functions

The spectral functions allow extracting single values, maxima/minima values, areas and parameters of a linear least-squares fit calculation from spectral data and inserting these values to a formula.

The following functions are available:

Table: Functions for various evaluations

Function	Calculation
YVal(WL)	Ordinate value at the given abscissa "WL"
AVal(WL)	Absorbance (A) ordinate value at the given abscissa "WL". %T data are transformed; error with other ordinate modes.
TVal(WL)	Transmittance (%T) ordinate value at the given abscissa "WL". Absorbance data are transformed; error with other ordinate modes.
RVal(WL)	Reflectance (%R) ordinate value at the given abscissa "WL". Error with other ordinate modes.
YMax(WL1|WL2)	Ordinate maximum in optionally given abscissa range "WL1", "WL2"
YMin(WL1|WL2)	Ordinate minimum in optionally given abscissa range "WL1", "WL2"
YPeakMax(SW|WL1|WL2)	Ordinate value of peak maximum in optionally given abscissa range with threshold value „SW"
YPeakMin(SW|WL1|WL2)	Ordinate value of peak minimum in optionally given abscissa range with threshold value „SW"
XMax(WL1|WL2)	Abscissa value of maximum in optionally given abscissa range
XMin(WL1|WL2)	Abscissa value of minimums in optionally given abscissa range
XFor(Ord|WL1|WL2)	Abscissa value of ordinate value „Ord" in optionally given abscissa range
XPeakMax(SW|WL1|WL2)	Abscissa value of peak maximum in optionally given abscissa

Function	Calculation
	range with threshold value „SW“
XPeakMin(SW| WL1|WL2)	Abscissa value of peak minimum in optionally given abscissa range with threshold value „SW“
Area(WL1|WL2)	Area under curve in optionally given abscissa range
Area(WL1|WL2|WL3)	Area under curve in optionally given abscissa range under curve with subtraction of ordinate value at abscissa „WL3“
Area(WL1|WL2|WL3|WL4)	Area under curve in optionally given abscissa range with subtraction of ordinate over 2 base positions “WL3” and ”WL4”
YMean(WL1|WL2)	Average ordinate value in optionally given wavelength range
XStart()	Abscissa start value of spectrum
XEnd()	Abscissa end value of spectrum
Spectrum(Parameter)	Value of given spectrum parameter, e.g. DataInterval. Further parameters see below.
SpecFactor()	Dilution factor or sample thickness of spectrum
SpecComment()	Description (info) line of spectrum (of use only, if just a figure given)
Slope(WL1|WL2)	Slope of the linear least-squares fit calculation in optionally given abscissa range
Intercept(WL1|WL2)	Intercept of the linear least-squares fit calculation in optionally given abscissa range
ResidError(WL1|WL2)	Residual error of the linear least-squares fit calculation in optionally given abscissa range
CorrCoeff(WL1|WL2)	Correlation coefficient of the linear least-squares fit calculation in given abscissa range

WL<number> represents a wavelength value. The vertical line is the pipe symbol.

Note: *The pipe symbol (vertical bar) can be generated by the combination of keys [AltGr] + [<] or by [Alt] + [124] (Holding the [Alt] key, while entering the number 124).*

Abscissa ranges are optional; when no values are given the full spectrum range is used. Brackets and the peak threshold value must not be omitted.

Available options with numerical contents for "parameter" of the *Spectrum(Parameter)* variable are:
DataInterval, Wavelength, OrdinateMin, OrdinateMax, CycleNumber, NumberofCycles, CycleTime, TimeOfThis Run, Slit, Temperature, ActualTemperature, SolutionVolume.

Example: The parameter line E:ymax()<Tab> Max. spectrum ord. value<Tab>: [2.3] <Tab>Maximal spectrum ordinate value will output the spectrum maximum value.
Example: E:xpeakmax(0.01\|400\|500)-xpeakmax(0.01\|400\|500)#1<Tab>Calculation 1<Tab><Tab>Calculation 1 will reference the position of a peak against that of the first spectrum of the series.
*Example: E:Ymax(360+Spectrum(DataInterval)*0.6\|400) delivers the highest ordinate value in the range of >360 to 400 nm. The 360 nm position is expliceitely excluded as requested in some norms.*

Use of Non-Numerical Spectrum Parameters in Conditional Outputs

Expressions as *Spectrum(Name/OrdinateValue/Comment)* can be used in the output of logical operators; see above.

ExampleE: m01(YVal(m03(500))#1) > m02(YVal(m03)#2) [Spectrum(Name)#1 has higher ordinate value at m03 nm (m01[1.3] Spectrum(OrdinateMode)#1)][Spectrum(Name)#2 has higher ordinate value at m03 nm (m02[1.3] Spectrum(OrdinateMode)#2)]

Calculations with multiple spectra

Calculations that apply to several calculations within a group of spectra are definable with an attached $<number>, respectively #<number>.

A required spectrum of the graph or within a series of measurements can be addressed in an absolute manner by an attached $<number>. *Example: E:xpeakmax(0.01|400|500)-xpeakmax(0.01|400|500)$1<Tab>Calculation 1<Tab> ….*

This will be generate the difference of peak position to the first spectrum of the series for each following sample spectrum.

Alternatively, a relative designation is possible with #<number>. *Example: E:xpeakmax(0.01|400|500)#2-xpeakmax(0.01|400|500)#1<Tab>Auswertung 1<Tab> …*:

This will generate the above difference for every second spectrum in respect to its previous spectrum.

When the required spectra are measured, the software will delete the error messages of missing reference spectra.

Parameter Calculation Results in Arithmetic Expressions

Arithmetic expressions also can utilize calculation results, like color values or transmission coefficients. This option allows defining calculations with result values, deciding on result values oder combining the results of different samples, e.g. for an average calculation. See the definitions for averages in the parameter definition file.

The result values are addressed by the *ResultTable* parameter. To address the correct result, the result output must be imagined as a table. This table has the rows p = 0 to n (with n evaluated spectra) and the columns q = 1 to m+2+x (for m selected calculations; the x additional rows are due to the fact that several parameters have more than a single result value).

Tip: *With executing the template Copy Results to Clipboard (see Data Handling Templates* 8-12*) and pasting the table into a spreadsheet program, the generated result table can easily be visualized.*

The initial *ResultTable(p,q)* variables are defined as:

ResultTable(0,1) Text „Spectrum“	ResultTable(0,2) Text „Description“	ResultTable(0,3) Designation of evaluation 1	ResultTable(0,4) Designation of evaluation 2
ResultTable(1,1) Name of spectrum 1	ResultTable(1,2) Description of spectrum 1	ResultTable(1,3) Result value of spectrum 1: evaluation 1	ResultTable(1,4) Result value of spectrum 1: evaluation 2 or second value of evaluation 1

ResultTable(2,1) Name of spectrum 2	ResultTable(2,2) Description of spectrum 2	ResultTable(2,3) Result value of spectrum 2: evaluation 1	ResultTable(2,4) Result value of spectrum 2: evaluation 2 or second value of evaluation 1

Example: The variable ResultTable(2,4) stands for the second result value of the the second spectrum to be evaluated.

Spectrum numbers are defined cyclically; i.e. if all applied numbers have been treated, numeration starts again with 1. If only 1 is used, this always refers to the current spectrum.

Note: *The principle requires that the original calculation results referenced by the ResultTable variable actually are generated and output. In the parameter definition file, the original calculation must be located before the ResultTable reference. Otherwise these values are not available. A calculation parameter must generate only a numerical value that is released from any prefixes and suffixes. Observe that comment lines in the report have to be counted as a row.*

Important:

The *ResultTable(p,q)* mechanism relies on a fixed list of calculated results. Whenever a calculation parameter is added or deleted, mapping of the *ResultsTable* parameter will be wrong.

Alternatively a result value can also be referenced via the *ResultTable* variable with the more extended syntax:

ResultTable(<spectrum name>,<short text> +/- n) or
ResultTable(p,<short text> +/- n) or
ResultTable(<spectrum name>,q), *(+/- n is optional)*

where *n* is an optional integer to switch to a succeeding value. The *spectrum name* and the parameter *short text* must be put into arrowed brackets. It is important that the parameter *short text* is identical to the short text within the referenced definition line.

Example: The expression E:(ResultTable(1,<tVIS (EN 171)>)+ResultTable(2,<tVIS (EN 171) >))/2 calculates the average Luminous Transmittance of samples 1 and 2.The Luminous Tranmittance calculation must be in the list of evaluations.

The advantage of this syntax is that the position of the referenced definition line can be changed without the need to modify the *ResultTable* definition.

As long as not all referenced spectra are measured for the *ResultTable* parameter of an expression, this calculation parameter will give a syntax error message. This error message(s) will be cleared, after the expression with a *ResultTable* variable has been evaluated successfully.

Note: *The spectrum file names ResultTable(1,1);(2,1);etc. and the spectrum descriptions ResultTable (1,2);(2,2);etc. are not usable in arithmetic expression. However, they can be inserted into a comment line.*

Ask Function

It is possible to integrate user queries into the calculation parameter lines via the Ask function. While the report is generated, the Ask function opens a text entry box, which requests the operator to make an appropriate entry, such as a specific numerical entry.
The syntax is: **Ask(text|min|max|default)**

The section “text” is used in the entry box as the user query. A typical request could be: **Please enter the weight of sample taken**.

Example: The parameter line E:Ask(Please enter the sample's water content [%]: |8|20|15) <Tab>Water content entry<Tab>: [2.1] %<Tab>Sample's water content queries the user to enter the water content as a figure. It offers the value "15" as the default entry for the user input and checks the entered value xx for the range 8 – 20. Outlying entries are rejected. The entered value is shown as: Sample´s water content: xx %

A figure entered for the ask function can be used in the current or in a following calculation via the ra variable (see following section).

Memory Variables

There are 2 options within a report layout to store numerical values: **ra** variables and **m** variables.

ra Variables

The **ra** variables (see above: **Ask** function) store a user-entered numerical value for later usage in a calculation expression. Up to 25 values can be hold with the variables **ra1** to **ra25**. The **ra** variables can be applied repeatedly.
Example: E:ask(Number input)+ra1<Tab>ra Example<Tab><Tab>Double of Input adds the input value to itself.

The ordering of **ask** variables corresponds to the order of generation of the **Ask** parameter.
The **ra**<number> variables should not be used with spectral functions. Use the **m**<number> variables instead.

m Variables

The **m** variables **m01** to **m99** allow transferring numerical values from one formula to the other. For this purpose the formula expression has to be defined as **m**<number>**(formula)**.
Example: E:m01((yval(500)+yval(550))/2)<Tab>Example Storage<Tab>: <Tab>Example Storage calculates the average of the ordinate values at 500 and 550 nm and stores the result as memory variable m01.

The variable can be used in a subsequent calculation.
Example: E:log(m01)<Tab>lg average<Tab>: [1.3]<Tab>Logarithm of stored average valuecalculates the logarithm of the average as calulated and stored in the above example.

This option allows you to dissect complex expressions. This will simplify the definition and the error tracing of calculations.

Examples

A few example are shown, which can be run with the spectrum **demo.dsp**, which is installed with the software. The spectrum should be loaded twice to the graph. Add the lines of interest to the parameter definition file **VL_ColorCalc.dta** in the Data directory with the Windows editor/ notepad and re-start the software.

On request we are happy to give you further support. Contact ***ascanis***.

1 – Readings at Defined Wavelengths

The measured spectra can be evaluated regarding readings at defined positions, peak maxima

and minima, general maxima and minima or integral values with an optional baseline subtraction.
Example:
the expression

100_001_001"Tab"E:xpeakmin(1|650|700)"Tab"Peak Minimum Position"Tab": [3.1] nm"Tab"Position of Peak Minimum in the range 650-700 nm

will output the wavelength position of the peak minimum (threshold 1) in the range of 650-700 nm.

2 – Evaluation Using Mathematical Equations

The values derived from the 1st example can be treated by mathematical expressions. The expression can include basic arithmetics, several levels of brackets and functions like **log**, **abs** or **sin**. Example:

100_001_010"Tab"E:log (xpeakmin(1.0|650|700)+100)"Tab"Log of Peak Min Position"Tab": [1.3]"Tab" Log of Position of Peak Minimum in the range 650-700 nm

3 – Logical Decisions

The results can be used to make logical decisions. Example:

100_001_020"Tab"E:abs(xpeakmin(1.0|650|700)-680)<=3[In tolerance][Out of tolerance]"Tab" Check peak range 680 nm"Tab""Tab" Peak Position Check (Range 680 +/- 3 nm):

The expression will test the position of the peak minimum to be at 680 +/- 3 nm.

4 – Using the Ask function

When user entries are required for the calculation or decision, they can be requested by the ask function. Example:

100_001_030"Tab"E:xpeakmin(ask(Enter threshold|0|5|2)|650|700)"Tab"Peak Minimum Position"Tab": [3.1] nm"Tab"Position of Peak Minimum in the range 650-700 nm

This will open a user query, which prompts the user to enter a threshold for peak detection. The default value for this entry will be 2, the allowed range will be 0 – 5. The according peak minimum position in the range of 650 – 700 nm will be output.

5 – Repeated User Entry

When a user entry is to be used repeatedly in an expression it can be repeated through a **ra** <number> variable. Example:

100_001_040"Tab"E:ra1"Tab"Treshold Entry"Tab": [1.1]"Tab" Applied user entered threshold

outputs the threshold for documentation as entered by the user.

6 – Transferring Values to other Expressions

Result values can be transferred to other expression through the **m**<number> variable. Example:

100_010_001"Tab"E:m01(xpeakmin(1|650|700))"Tab"Detection of Peak Minimum Position"Tab": [3.1] nm"Tab" Position of Peak Minimum in the range 650-700 nm

100_001_01"Tab"E:yval(m01)"Tab"Output of Peak Minimum Value"Tab": [1.3]"Tab" Ordinate Value of Peak Minimum in the range 650-700 nm

will store the peak minimum at a storage position. The second expression evaluates the corresponding ordinate value.

7 – Calculations for More than One Spectrum

It is possible to calculate with data of several spectra. The spectrum has to be identified with the #<number>. Example:

100_010_10"Tab"E:abs(xpeakmin(1.0|650|700)#2- xpeakmin(1.0|650|700) #1)"Tab"Difference Peak Minimum Positions"Tab": [2.1] nm"Tab" Difference Peak Minimum Positions of 2 Spectra

will calculate the difference is peak position of spectrum 2 compared to spectrum 1 in a series.

8 – Referring Spectra to a Reference

Within a series of spectra it might be necessary to refer all spectra to a reference. Example:

100_020_01"Tab"E:xpeakmin(1.0|650|700)-xpeakmin(1.0|650|700)$1"Tab" Difference Peak Minimum Positions to 1"Tab": [2.1] nm"Tab" Difference Peak Minimum Positions to Spectrum 1

will calculate the difference of peak minima for each spectrum compared to that of the reference spectrum, which is measured as the first spectrum.

9 – Using ResultTable parameters

ResultTable parameters allow integrating calculation results into arithmetic expressions. Example:

100_030_01"Tab"E:(ResultTable(1,3)+ResultTable(2,3))/2"Tab"Average Parameter 1"Tab": [3.3]"Tab"Average Parameter 1

will calculate the average of the first selected calculation parameter (whatever that is) for 2 consecutive spectra.

8.10.5 Sample Classifications

Samples can be classified into groups according to their calculation results by extending the basic parameter definition. This done by adding the expression *class<TableFile>* (no space between *class* and < >) after the output of result(s).

Example F:sunlight.dat"Tab"Sample Classification"Tab"[3.1] class<TableFile>"Tab"Classification Result:

The file T*ableFile* holds the class definitions in a tabular form, see below.

Then, instead of the result value(s), the class designation is output or a default text, if the sample cannot be assigned to one of the classes. In order to have the value(s) as well, an additional parameter definition line must be applied.

The classification may be multi-dimensional, i.e. it can be referenced to several output figures, see the example below.

The classification limits are summarized in the classification table file *TableFile, which* consists of 3 sections with a given syntax:

1. The header line must start with the the keyword *Range* followed by an optional commentary text.

2. The data section consists of a number of lines that represent a class each. Each line has a class designation and the corresponding result range(s) of the class (upper and lower limit for each classification figure). ▼ *ExampleLow protection "Tab" 75 100*
   The class designation must be separated by "Tab" character; the numerical values can use a "Tab" or a space character for their separation. Figures must use the point as the decimal separator.

3. A default text is output, if the calculated result(s) do not fit to any of the listed class definitions. The last line is the default text line; it starts with the default text and is terminated by "Tab"* (star character).

A parameter line for classifying a sample color to 3 red definitions (designations and limits only just examples) via the sample's Lab-values would look like this:

100_001_001 "Tab" C:L-d6510grd.dat "Tab" Red classification "Tab" [3.1] [3.1] [3.1][0.0] [0.0][0.0]
class<RedClasses.txt> "Tab" Result of red classification:

Note: *The output format definitions [n.m] (except [0.0]) and the class<> definition must each be separated by a space.*

The corresponding classification table file *RedClasses.txt* may look like this:

Line of classification table file	Meaning
Range Red classification via Lab-values	Header line

red "Tab" 50.0 100.0 75.0 120.0 -10.0 10.0	Data section: class 1, definition of red sample
medium red "Tab" 45.0 80.0 40.0 75.0 -10.0 10.0	Data section: class 2, definition of medium red sample
light red "Tab" 30.0 45.0 10.0 40.0 -10.0 10.0	Data section: class 3, definition of light red sample
*Not classified as red/medium/light red "Tab" **	Default text line: sample not within one of the above classification ranges

"Tab" stands for the tabulator character.

The file is generated by the Windows notepad/editor and it must be present in the software's Data directory. Classification table files included with the software's install set can be encoded and have the .dat file extension.

With a sample of Lab=40/38/0, the parameter will be output as:

Result of red classification: light red

See the software's parameter definition file for another example that classifies a sample to the basic colors.

Note: *Output prefixes or suffixes cannot be applied in the format section of the parameter definition line, if a classification is included.*

Note: *When the data have been classified successfully, the classification process is terminated. General classifications or those of higher priority therefore should be in the top lines of the table.*

In addition to the result values of the specific calculation, results of other calculations can be introduced via *ResultTable()* variables that is placed in curly brackets. The above example could be extended e.g. as

C:L-d6510grd.dat "Tab" Red classification "Tab" [3.1] [3.1][0.0][0.0][0.0][0.0] {ResultTable(1,<tVis (EN 171)>)} class<RedClasses.txt> "Tab" Result of red classification:

Thus, the light transmittance of the sample could be included as a further criterion in the classification. The classification table file must be extended accordingly with the upper/lower limits for this parameter.

Important: For a reference to a ResultTable() variable, the referenced result value must actually be contained in the report.

8.11 Report Configuration

The software generates reports showing the spectrum graph and the evaluation results. The report format is predefined.

Alternative Report-Template with Logo Function

To integrate a logo symbol to the report, replace the file *VL_ColorCalc.rpx* of the **Data** directory with the file of the same name in the */tools* directory. With the page layout template, a graphics file of the name *logo.jpg/bmp/tif* in the same directory is placed in the report header section. The size of the logo must be adapted to the reserved space.

ascanis additionally offers the **Reporter-SPX** application software, which provides a high level of freedom in the presentation of the graph and the page layout of the report. You install **Reporter-SPX** as an independent application, which additionally gives you a powerful tool for the generation of customized analytical reports based on saved data.

Additional Features with Reporter-SPX

Installation of **Reporter-SPX** opens additional functions:

- Clicking the right mouse key in the graph area opens the **Chart Control Properties** window. This window contains a multitude of functions that allow you to configure the graph area, such as spacing of grid lines, background color of the diagram, or the assignment of spectral curves to the left or right Y-axes. The modified settings can be stored and act to the screen graphics and the report graphics. See: *Graph Layout* 8-38
  All functions of the **Reporter-SPX Chart Control** window are described in the accompanying *Operator's Manual*.

- The additional **Page Designer** command in the **Options** menu opens the **Page Designer** module of **Reporter-SPX**. **Page Designer** determines the page layout of the report. You can select the size of the diagram, add your company's logo, insert additional variables and text information strings, etc. See: *Page Layout* 8-39
  See the *Reporter-SPX Operator's Manual* for more details.

- Additionally, an **Export** function is available in the **File** menu. In addition to the standard export of a report in PDF format, the **Export** function supports various formats. See: *File Menu* 5-3 *and Export* 8-37
  Details of the command are described in the *Reporter-SPX Operator's Manual*.

- **Reporter-SPX** allows creating additional templates with integrated VBA-scripts for the **Data Handling** or the **Measure** menu, where the templates appear as menu items. The templates reside in the Data directory and they must have the filename <Name>.MS.rpx (Measure menu) or <Name>.DH.rpx/<Name>.SC.rpx (Data Handling menu).*Example: With a filename mean.SC.rpx the corresponding menu command "mean" will be shown after restart in the data Handling menu.*

  With the templates with integrated scripts further data evaluations of the spctra displayed in the graph or other functions are made possible. Some examples are available in the /Tools directory of the program CD. See section *Data Handling Templates* 8-121.

  With the installation of Reporter-SPX, further examples are installed. Further templates can

be user-generated via the **Page Designer** program section or can be developed by ***ascanis*** on request.

Generating Layouts

Reporter-SPX uses special graph layouts (***.oc2**) and page layouts (***.rpx**).

- The standard graph layout template of the software has the filename *VL_ColorCalc.oc2* and is located in the Data directory. Reporter-SPX allows modifying this template. Any changes you make to the graph layout template influence the graphics screen presentation and the reports for all methods.

  Also, you can also define a method-specific graph layout. This must have the same root filename as the selected method and must be saved in the method directory. See: *Preferences* 5-12

- Similarly, the standard page layout template of the software has the filename **V***L_ColorCalc.rpx* and is also located in the Data directory. Any changes you make to the page layout template via the **Page Designer** influences the reports for all methods (unless you have defined method-specific page layouts).

  You can also define a method specific page layout. This must have the same root filename as the selected method and must be saved in the method directory. Since also calculations and decisions can be involved, a print preview of the report is generated automatically after a measurement, if a method specific page layout is employed. *Example: For the method Test1.mol, a method-specific graph layout would have the filename Test1.oc2 and a method specific page layout would have the filename Test1.rpx. Both files must be present in the method directory.*

The sample path length that is integral to the spectrum is assigned to the *SpectrumFactor* control in the **Page Designer**.

- A further page layout *TextReport.rpx* is applied for plane text output, e.g. with the **Show method** function.

Special Hints for Working with Reporter-SPX

With **Reporter-SPX** peak labeling within the report graph is supported. To use this feature, the graph layout must be defined with the **Reporter-SPX** user interface, because only here the options to define peak labeling are available.

Rather than the standard presentation of the calculations, the **Page Designer** allows placing selected parameters at any arbitrary position and in an individual format into the report with the **ResultTable** (column,row) variable. The example report layout **ResultTable.rpx** that is installed with the software shows the procedure.

If the graphics include both the spectrum corrected for the pathlength and the original spectrum following pathlength correction, do not forget to distinguish the parameters with the **#1** and **#2** extensions.

See the *Reporter-SPX Operator's Manual* for all details of the described **Chart Control** window and **Page Designer** options.

8.11.1 Export

The **Export** command is only available with additionally installed **Reporter-SPX** software. See for more details in the *Reporter-SPX Operator's Manual*. See: *Report Configuration* 8-35

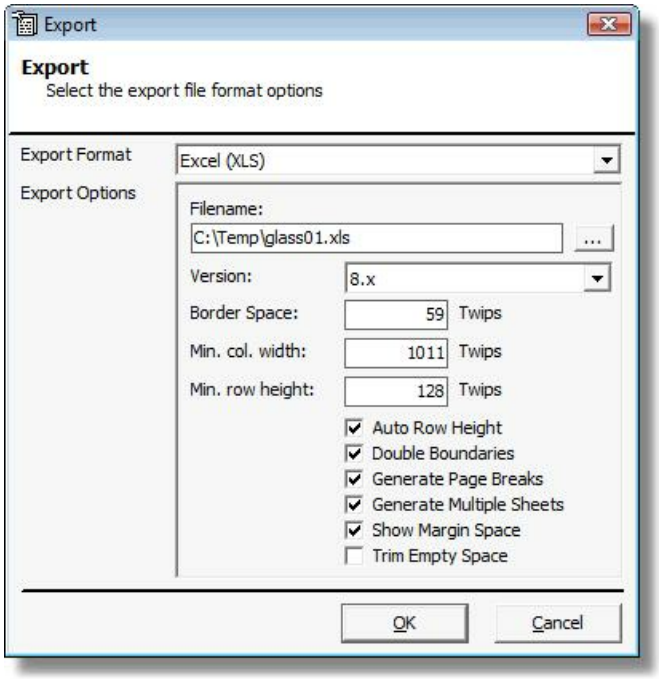

Figure: Export window

The **Export** command allows you to generate report files in a selectable format and to save them in a selected directory. Clicking **Export** opens the **Export** window in which you can select the file type, path and name, and a range of other options.

1. Select the requested file format in the **Export Format** drop-down selection box.

Table: Data Formats for Export

Data Format	Description
RTF (Rich Text format	This is a program-dependent format for word processing.
PDF (Portable Document Format)	This is a very widely used format for transferring documents. You can open pdf files with the Adobe Acrobat Reader, which is available free-of-charge.
HTML (Hyper Text Markup Language)	This is a page description language that finds application in particular for Internet Web pages. This format is displayed by web browsers and can also be imported by a number of word processors.
TIF (Tagged Image Format)	TIF files are loss-free compressed bitmap graphics files. You can open and modify TIF files using proprietary graphics programs.
XLS	Microsoft® Excel Format.

2. The first entry in the **Export Options** dialog is the filename and path.
   The path displayed is the path currently selected in **Options**, **Preferences** and the filename is that of the current spectral data file, or of the first file if multiple spectra are displayed.
   To change to a different path or filename click the browser button (**...**) to the right of the proposed filename.

   When you select PDF or HTML, further dialog windows are presented that allow you to make additional entries that are specific to these file formats.

3. After completing selections, click **OK** to export the file to the selected location.

8.11.2 Graph Layout

This function is only available with the additional **Reporter-SPX** software. See for more details in the **Reporter-SPX** documentation. See: *Report Configuration* 8-35

You configure the graph layout in the **Chart Control Properties** window. To open this window, right click in the graph area. The **Chart Control Properties** window contains a multitude of functions that allow you to configure the chart area. Entries or changes you make are displayed immediately in the chart area, when you complete the entry or as soon as you click **Apply**. You can thus easily try out the various options.

Note: *For numerical entries in the **Chart Control Properties** window you must use a period (.) for the decimal position, even if a comma is selected as the decimal symbol in Windows.*

The settings you can make in the **Chart Control Properties** window are divided in 12 pages:

Table: Parameters for graph layout

Parameter	Function
Control	Governs the general appearance of the chart area.
Axes	Defines the axes of the spectral graph.
ChartGroups	Defines various chart groups.
ChartStyles	Defines how the spectral data are displayed.
Titles	Governs the appearance and position of titles.
Legend	Defines the appearance and position of the legend box.
ChartArea	Determines the appearance and position of the chart area in the report.
PlotArea	Defines the properties of the plot area.
ChartLabels	Defines the appearance and position of text labels in the plot.
View 3D	Allows a three-dimensional presentation.
Markers	Defines the appearance of marker lines.
AlarmZones	Allows marker bands to be placed behind the plotted data.

When you click on a tab, the respective page is moved to the front. Each page has a number of inner tabs, which access specific property pages. If not all inner tabs are visible, arrows are presented at the right side of the tab bar. Use the arrows to shift the tabs to left and right.

Graph Layout Chart Options

The **Chart Options** window is presented as soon as you close the **2D Chart Control Properties** window or save the graph layout.

Axis scale tab

You use this tab to set the maximum and minimum vertices (corner points) of the three possible axes.

Full	The respective vertex (corner point) of the axis corresponds to the smallest or largest data point to be displayed. If **Full** is selected for all vertices, the curves are displayed at maximum size.
Rounded	The vertex of the respective axis is selected automatically such that it has a significant or rounded value.
Fix	The current settings of the axis vertices are saved. The axes are not adjusted to the data points. With this option, spectra in a series are always displayed with the same scale, facilitating comparison of the data.

Note: *If the second spectrum in a series is to be automatically assigned to the right-hand Y2 axis,* ***Y2min*** *and* ***Y2max*** *must be set to* ***Fix****.*

Axis title tab

This tab allows you to select the axes units (e.g., nm, A, etc.)

Automatic	The axes units are automatically taken from the spectral data. Any changes that were made to **Axes/Title** in the **2D Chart Control Properties** window are ignored.
Fix	Changes made to **Axes/Title** in the **2D Chart Control Properties** window are saved.

Legend tab

The tab offers the **Show spectrum description** check box. If selected the graph legend box will show the data file description text for each data file. It may be preferable not to show the description if there are space limitations.

8.11.3 Page Layout

The definition of a report page layout is only possible, if the additional **Reporter-SPX** software is installed. See for more details in the **Reporter-SPX** documentation. See: *Report Configuration* 8-35

The command starts the program section **Page Designer**. You close **Page Designer** window using the standard buttons in the window header.

Page layouts are stored as files with the extension **.rpx** in the method directory and they are loaded or saved via the **Open** or **Save** commands in the **File** menu.

The **Page Designer** window shows the report area, where you configure the page layout, in the center of the window. The report area has top and side rulers. The report area is structured. You use the horizontal gray section bars to separate the various sections of the report. Each report section (e.g., **ReportHeader**, **GroupHeader1**) has specific properties, which you can set in the **Property ToolBox**.

Visual elements (known as controls) are displayed in the report area. Each chart element has a name and type-specific properties. A list of the available chart elements together with the structure of the layout is presented in the navigation view via the **Explorer** command in the **View** menu. Properties of the active visual element are displayed in the **Property ToolBox**.

You can select a new visual chart element either from the left **ToolBox** or from the left variables selection box. Current visual chart elements can be modified in a number of ways. You click the requested chart element so that it is surrounded by grab handles.

Editing and formatting functions include:

- Copying, pasting, dragging, deleting, and resizing with the mouse or keyboard.
- Editing the properties in the **Property ToolBox**.
- Commands from the context menus (right-click the chart element).
- Commands from the **Edit** and **Format** menus.

Note: *You must save a new page layout before it is available for the software. You do not have to close **Page Designer**, however.*

8.11.4 Reporter-SPX – Scripts in a Page Layout

Page layout templates may include VB scripts for dedicated purposes. They are defined via the Reporter-SPX software. For that, dedicated functions allow accessing the software's data and results, graph and results area or format and I/O options. Thus it is possible to set up for example specific data handling routines, instrument control or export functions. See for example the templates described in *Data Handling Templates* 8-12.

The Reporter-SPX manual contains notes and example for the script functions. Contact ***ascanis*** for further information and support.

9 Data Formats and Import/Export of Spectra

A data files comprise a single spectrum. By default, the files have the file extension **.dsp**. The files are text files with a header holding general information like spectrophotometer settings, data and time of recording, spectrophotometer details, etc. The header is followed by the data section. A detailed definition of the data format is given in the CD's directory */tools*.

Spectra can be loaded and stored also in alternative data formats, see below and the section about the external spectrum converter.

Also, the software utilizes the file extension **.mol** for method files and **.lol** for sample list files.

With the installation, the software registers the method file type. Thus it becomes possible to start the software by clicking on the method file directly with the selected method. This can be also done via a desktop link for a method file.

Loading spectra

The **Load spectrum** command will read spectrum files and data set files of different formats. All formats are text based.

Table: Supported spectrum data formats

Import of Spectrum Files

Import of Tabular Format Data

When importing tabular data, the software requires data with the following structure:

- Up to 25 header lines with the sample description and abscissa/ordinate units
- Table of abscissa/ordinate data pairs. A list separator character separates the abscissa/ ordinate data.

Such a text format is typical for ASCII data storage in the txt or csv format of Microsoft Office Excel®.

Header lines are recognized by the fact that the first character is not a figure. If the last of the header lines contains the list separation character (see below), the information before and after that character is interpreted as the name of the abscissa and ordinate units, e.g. *nm;%T*.

If such a definition is not present, **nm** is applied as the abscissa unit, if the first abscissa value is larger than 150. **A** (absorbance) is used as the ordinate mode, if all data are <6; otherwise % T is used.

If the ordinate is designated **Abs** or **Absorbance**, it is changed to **A**.

IMPORTANT:

Some csv-spectrum sources use ordinate designations like T, R or T%. When importing such a spectrum with ordinate values >1.25, the software assumes that actually these data are %T / %R. The ordinate mode is changed accordingly. If all spectrum values are <1.25, the original ordinate designation is maintained.

The other header lines are added to the sample description. Text that follows the data section is interpreted as audit trail information.

The list separation character is expected to be as set in the Windows configurations for the current user. If this standard list separator character does not appear, a comma, tab or space is searched. The list separator is recognized by occurring only once in a data line.

The decimal character also is expected to be as set in the Windows settings. If numbers cannot be recognized, other decimal characters are checked to produce meaningful data.

Further separator characters (empty columns) and empty lines below the data range are ignored.

A standard decimal number format is expected. But it is also possible to have numbers in an exponential form.

The abscissa values can be arranged in ascending or descending order. A constant data interval is not required – if so, the data are interpolated to the lowest occurring data interval. Beforehand, abscissa data are rounded to the 10th position after decimal point.

The imported csv file may also hold several spectra in the form x y y y or x y x y.

The import file may be based on ANSI or standard Unicode character sets.

Tip: *When you import data files with its specific file extension repeatedly, it is possible to include this file extension in the list of default extensions offered by the* ***Load Spectrum*** *command. This is done by defining the following line in the* ***[Configuration]*** *section in the software configuration file;* see *Options in the Configuration File* 8-3

[Configuration]
SpectrumReadTypes = .<specific file extension>

Example

As an example for the import of tabular data, spectra generated by a spectrometer software of a different brand can be imported. The spectra have the format:

"Storage 151148 5GI205 - RawData -D:\Applikationen\Hilfe\File_040622_R.spc"
"Wavelength nm.","R%"
190.00,6.758
192.00,6.671
194.00,6.532
196.00,6.421
…

JCAMP Spectrum Import Format

The JCAMP format is a text format to exchange spectral data among different software platforms. The files may have different file extensions, like **sp**, **dx** or **jcm**. The variant handled by this software consists of a header and a data table. The header contains various general information designated by a leading ##. *Example*

##TITLE= Azorubin, 0.9384mg/100ml
##JCAMP-DX= 4.24
##DATA TYPE= UV/VIS SPECTRUM

This information is transferred to the spectrum information as far as possible; other information is transferred to the audit trail block.

The data section follows after the factors for abscissa and ordinate values and the internal format definition. Each line includes an abscissa value and the following ordinate values. *Example*

```
##XFACTOR= 1.00
##YFACTOR= 0.00000011920928955078
##XYDATA= (X++(Y..Y))
700.000000   11743   11743   11743   11743   11743
695.000000   11743   11743   11743   11743   11743
690.000000   11743   11743   11743   11743   11743
...
##END=
```

The data section is terminated by an *##END=* line.

The import routine will also accept JCAMP-DX files, which have more or less ordinate values within a data line.

The format may contain a series of spectra. According to JCAMP 4.24 definitions, this is defined at the beginning of the file via the line

##BLOCKS=n (n: number of the following complete data sets)

Note: *As there are many options to design JCAMP-DX files, JCAMP spectra from other software packages may not be imported, if this standard JCAMP-DX spectrum format used with this software is not observed.*

Spectrum Export in csv or JCAMP Format

As an alternative to storing spectra in the software proprietary format, the **Save** as function in the **File** menu and in the **Spectrum** information window allow saving a spectrum in the **csv** format or the **JCAMP** format.

Note: *Storing spectra in the **csv** or the **dx** format will not include all measurement parameters. These will only be kept with the standard **dsp** format.*

If you want to store recorded spectra automatically in the **csv** or the **dx** format, this can be defined in the configuration file. Use the following line to the **[Configuration]** section in the software configuration file:

[Configuration]
SP_EXT = .<filename extention> (<filename extention>: **csv** or **dx**)

With this setting the standard format for spectrum storage will be the applied format instead of the proprietary **dsp** format.

Format of the Generated csv File

The list separator character is used as set in the Windows configuration, if not set, a semicolon is used. Also the decimal point is applied as set with the Windows configuration.

As a default, the **csv** format has 2 leading text lines. The first line summarizes a number of spectrum parameters separated by the list separation character. The second line holds the table headings, e.g. **nm**; **%T**. Other options can be configured by the **ExportFormat=** parameter within the **[Configuration]** section of the configuration file,see *Options in the Configuration File* 8-3.

Format of the Generated JCAMP File

The export JCAMP-DX format is as described above. It follows specifications version 4.24. As a default, the format has one ordinate value per data line. This can be modified by a definition within the software configuration file: Use the parameter **JCAMPFormat=**<number> in the **[Configuration]** section, where <number> is the number of ordinate values within a data line, see *Options in the Configuration File* 8-3.

Note: *As there are many options to design JCAMP-DX spectra, other software packages may not be able to import the specific JCAMP-DX spectrum format used with this software.*

Tabular csv-Format for Results

The **Export Results** command saves the results of the results space in a tabular csv-format. Compared to the screen presentation of the results, the orientation is changed from a line-by-line output to a column oriented order.

The schematic layout of the file is:

"Spectrum"	"Description"	Designation parameter 1	Designation parameter 2	Designation parameter 3	etc.
Name spectrum 1	Description spectrum 1	Result parameter 1 for spectrum 1	Result parameter 2 for spectrum 1	Result parameter 3 for spectrum 1	
Name spectrum 2	Description spectrum 2	Result parameter 1 for spectrum 2	Result parameter 2 for spectrum 2	Result parameter 3 for spectrum 3	
etc.					

Tip: This arrangement of results is also applied with the template Copy result table to clipboard. See Data Handling Templates 8-12.

Using an External Spectrum Converter

It is possible to use further data formats within the software. For that, an external routine for spectrum conversion can be added. The executable program file is stored in the program directory of the software under the file name

SPC_CONV_<process>_<name of file type>_<filename extension>**.exe**

where:

<process>	the required process: **R** (Read); **W** (Write/Save as); **S** (Save/automatic storage) (multiple entries are possible)
<name of file type>	the name of the external file type;
<filename extension>	the existing or requested filename extension

The additional file type is then additionally offered with the **Load Spectrum** or the **Save as**

command.

Contact ***ascanis*** if you intend to use this feature for specific data formats.

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10 Spectrometer and Accessories

Further sections of this chapter hold information on the various spectrometer models and accessories.

10.1 Thermo Scientific Spectrophotometers

Models Thermo Scientific GENESYS 20, Helios epsilon and SPECTRONIC 200 are not feasible to be used with this software.

GENESYS 10S and Compatibles

The spectrophotometers

GENESYS 10S Vis/ 10S Bio/ 10S, BioMate 3(S) and Evolution 60S

are recording single-beam or split-beam instruments (internal reference detector). GENESYS 10 (S) Vis has restrictions in wavelength range, data interval, spectra bandwidth and scan speed selection. The software does not offer reflectance modes.

Instruments of the GENESYS 'S' series use PC communication via USB port. The applied port has the designation *Spectrophotometer*.

Important:
The instrument keyboard cannot be switched off. As long as the instrument is under PC control the instrument keyboard should not be used. Otherwise the system may crash and erroneous data may result.

Important:
If the instrument does not display the main screen (but e.g. the utility screen) the software may partly malfunction.

For these instruments, a dedicated sipper accessory is not available. Instead, a PC-controlled sipper pump (Economy Sipper) can be employed to automatically sip samples. See *PC-controlled sipper pump* 10-10.

The spectrophotometers allow storing method and data files to a USB stick. However, these data are incompatible to the software except for spectra that are stored in the JCAMP-DX format.

Error Messages

When you start the software and the instrument is not yet switched on or is in the initialization phase, the error message will be:

No response from instrument on device com<number>**.**

When the instrument is not properly connected to the PC, the error message will be:

Error accessing communication port com<number>**. The system cannot find the file specified.**
Invalid port number.

Display and Standby

When the software controls the instrument, the instrument display shows the message (in local language, if selected as the instrument operating language):

Instrument is in Remote Mode
Press ESC to cancel.

During spectrum scanning the live display and the graph remain blank since the data are transferred to the software only when the scan is finished. (See: *Operating Toolbar* 5-2) The software messages the scan or the baseline correction run with an appropriate window; check the scan progress at the instrument's display. The instrument displays the message

Acquiring data ... <percentage> **% completed**.

After the end of the scan the graph is displayed and the live display is reactivated.

Note: *Data transfer can take up to several minutes, if a large wavelength range and/or a low data interval have been used.*

If the instrument is configured with a lamp saving standby time and if no measurement is done for 5 minutes, the software will quit communication. After the selected standby time the instrument itself will then go into the standby mode and will shut down the lamp. The software's live display shows ******* instead of an ordinate reading. However, use of an instrument function will immediately activate the spectrometer. See: *Configuration file* 8-3

Autozero/Baseline

An autozero/baseline run is required whenever the scan range or the data interval is changed. An autozero/baseline run is also required even if the data interval is a multiple of the previous value, or if the scan range is a restricted section of the previous range. Even though some instruments accept this, GENESYS 10S and compatible instruments return an error message. See: *Executing a Baseline/Autozero Run* 6-1

The spectrophotometer does not allow to autozero higher absorbance values. An error message *Cannot zero* is returned in this case. Remove the absorbing sample and restart the autozero.

Specific Parameters

The scan speed of the series of instruments is selected in three levels. (See: *Spectrophotometer Parameter Group* 5-15) With a 1 nm data interval, these levels correspond to:

Slow	approx. 400 nm/min
Medium	approx. 800 nm/min
Fast	approx. 1500 nm/min

The baseline correction run is always done with the lowest possible scan speed.
(GENESYS 10S Vis ca. 1500 nm/min and 800 nm/min for baseline correction)

A scan must cover at least 5 data points.

Cell Changer

GENESYS 10S and compatibles can be equipped with a 6-cell changer. The first position of the cell changer **B** is reserved solely for the blank and cannot be used for sample measurements. An autozero is always performed at this position.

An alternative cell holder (**Auto-3**) is offered for long-path cells. You can define the use of this holder in the **Preferences** command. This setting is valid for all applications. See: *Options Menu* 5-10

Note: *The **Auto-3**/**Auto-6** selection is offered also, if no cell changer is installed. In this case, the selection is irrelevant.*

After installing or removing the cell changer it is necessary to restart software and instrument so that the new configuration is detected.

Peltier Accessory

The Air-cooled Peltier accessory SPG 1A is an option for thermostatting rectangular 10 mm cells in the range of 20-60 °C for a measurement. The accessory does not require handling a thermostatting liquid. It is compatible to the GENESYS 10S series spectrophotometers, see below.

Evolution 200 Series

Evolution 201, 220 and 260 Bio are recording double-beam UV/Vis spectrophotometers with USB communication. An appropriate USB driver is installed automatically.

A local control version (with built-in screen) and a computer control version (without screen) are available.

Important:

When the Thermo Scientific INSIGHT® software is additionally installed on the PC, the resident Insight Launcher routine interferes with the communication by taking control of the spectrophotometer USB port. When VISION*lite* ColorCalc is started, the following message is shown:

Error accessing communication port COM ?. Port already open.
Please close all other software ....

In this case, end the InsightLauncher process in the Windows Task Manager. To remove the problem permanently, remove the corresponding registry entry or delete or rename the InsightLauncher executable, which is not required for instrument operation for either software.

Accessories

The Evolution 200 platform supports a number of Smart and/or electrically powered accessories, not all of which are supported by the VISIONlite ColorCalc software.

The following accessories are supported:

- All manual accessories – those which do not require an electrical connection to the instrument
- Smart 7-cell rotary changer
- Smart 8-cell linear changer
- Smart Sipper
- Integrating sphere ISA-220
- Integrated fiber optics module
- Evolution™ Peltier Thermostatting Accessory PCCU1, see below
- Hg Lamp

The following accessories are not supported in VISION*lite* ColorCalc software.

- Temperature probe
- Rapid mixing accessory
- Calibration and Validation Carousel

For these accessories, please use the INSIGHT software supplied with the Evolution 200 series instrument.

After installing or removing an electrical accessory it is necessary to restart the software so that the new configuration is detected.

Cell changer

Important:

For Evolution 200 series instruments with cell positioner, it is advisable to run a cell changer optimization after system setup and possibly also during operation. This routine re-defines the coordinates of the cell positions. In the **Open** window of the **Load Method** function, switch to the parent directory *Service* and load the routine *CellChangerOptimization*. Click **OK** to start the routine.

See also below *Warning Message with Cell Changer Start.*

Initialization and Communication

Initialization

After startup, the instrument requires several minutes for initialization. The exact time depends upon the precise model, with Evolution 201 requiring only ~2 minutes and Evolution 220 and 260 Bio requiring longer. If the software is launched during the instrument initialization process, the message **No response ...** or **Instrument is initializing ...** is shown. On local control versions of the instrument, INSIGHT software will launch automatically and the progress of the initialization is shown in the lowermost line of the instrument's screen.

Communication with Local Control Models

To establish communication between software and instrument of the local control version, after instrument initialization simultaneously press the keys **[2]** + **[4]** on the instrument's keyboard for 4 seconds. Alternatively, in the internal instrument software, choose **System Settings** > **System** . In the **Instrument Control** group, select **Computer**.

Thereafter, the message (Internal) **Instrument control is disconnected** is shown. This message may be disregarded. Then the lowermost line of the instrument's screen shows the message **Connected to PC**. The instrument's internal software may be operated, but does not

have access to the instrument any more. The software can also be closed.

Important:
For spectrophotometers of the Evolution 200 series the live display only shows approximate ordinate values, when the instrument is inactive. Thus the display can only be used as an orientation, but not for a sample reading. Use the **Manual Control** function to read sample ordinate values after executing **Autozero**.

Switching off the Spectrometer

To switch off the instrument, press the Power key and accept the Shutdown message of the internal operating system (local control version).

Operating the external Mercury Lamp

In order to operate the pluggable Mercury Lamp Calibration Accessory, the accessory can be attached, but must not be plugged-in, when the instrument is powered. However, with start of the software, the accessory must be plugged in so that the software can detect it.

Instrument Parameters

Slit

Model Evolution 220 is equipped with a variable slit. For the **Slit** setting (**Advanced Options** window) the standard choice is 1 or 2 nm spectral bandwidth (written as 1_nm, resp. 2_nm). Additional slit settings are adapted to specific accessories. Make sure to apply the appropriate setting.

Sphere	Maximized beam spot; used for integrating sphere measurements (15 nm bandwidth)
Fiber	Small round beam spot; used for coupling to light fibers (5 nm bandwidth)
Micro	Narrow beam spot for micro cells and micro measurements (Shortened rectangular beam with 2 nm bandwidth)
Blocking	Blocked beam for test purposes only

Important:
The **Slit** setting **Sphere** is only to be used with the ISA-220 accessory when measuring particularly dark samples (<10%T or 10%R). When using this setting, it is essential that the 1A screen filter supplied with the accessory be placed in the reference cell holder. Failure to use the reference beam attenuator will result in reference detector overload which will cause inaccurate readings.

Scan Speed

When high scan speed settings are selected together with small data intervals the system may not be able to reach the selected speed. The instrument will not return an error or alert in such a case so the method may show a higher scan speed than is actually used in the experiment: e.g. for the smallest data interval of 0.05 nm a maximum scan speed of appr. 150 nm/min is reached.

Integration Time

The software does not offer selection of an integration time. Instead the integration time is automatically set according to the selected **Scan speed**, i.e., if the scan speed is smaller than the maximum possible speed, the integration time is increased to the highest possible value.

Wavelength entry

The instrument can set wavelengths only in 0.2 nm increments. E.g. it is possible to use 500, 500.2, 500.4 nm etc.; but wavelength entries like 500.1, 500.3 nm etc. should not be done. When entering such a wavelength value an error message is given:

Error communicating with the spectrophotometer; Command WDR ???.? ; Answer: ?Error 3092

Another wavelength value has to be entered.

Wavelength Setting "0 nm"

For alignment and test purposes, the software allows entering a wavelength of 0 nm in **Manual Control** mode. The beams then have non-monochromic (white) light. See *Manual Control* 5-10.

Sipper

The instrument does not allow the sipper to be run permanently. Instead, when clicking the **Sip** button in the **Manual operation** or in the **Sample information** window, the sipper is activated for the maximal time possible. Thereafter it can be restarted by another click to continue sipping.

Cell Changer

A template routine to optimize cell changer positions is available in the *Service* directory, see above.

A message can be issued with the initialization of an accessory. See the *AccInitMessage* parameter: *Configuration file* 8-3.

Automatic Source Switch-off

The **ascapp.ini** configuration file allows a time for source switch-off to be defined. When the defined time has elapsed after a measurement, the lamp is switched off automatically. This is to limit lamp working hours and so to extend lamp life.

If no entry is done in the configuration file, the default switch-off time is 3 min. See: *Options in the Configuration File* 8-3.

Readings above 100 %R/T

The Evolution 2xx signal amplification is continuously optimized to achieve an optimal signal-to-noise ratio. Accordingly, readings substantially above 100 % or below 0.000 A may become erroneous by an internal data overflow. Therefore, a measurement is canceled with an error message for readings >125 %R/T or < -0.100 A.

Warning Message with Cell Changer Start

When operating the instrument with a cell changer, a warning message for the user is provided, if the cell changer starts ist movement. There is a risk of personal injury. A corresponding warning can be implemented for software operation with the *AccInitMessage*= configuration parameter. See: *Configuration file* 8-3.

Evolution 300

Evolution 300 is a scanning double-beam instrument for the entire UV/Vis range. It has various accessory options (see below). The instrument is available as a local control (stand-alone) version or as a PC-control version that only can be operated though a PC.

For establishing communication between software and instrument on a local control instrument, it is necessary to switch the instrument to REMOTE mode. Do this by pressing the REMOTE key on the spectrophotometer after the initialization is finished. If the instrument is not in REMOTE mode, the software will present the error message **No response from instrument**.

Note: *With Evolution 300, typically there are long reaction times in error situations.*

Note: *During REMOTE mode the keyboard is locked and the instrument's LC display only indicates REMOTE mode operation. To switch back to normal instrument operation, first exit the software and then press the [HOME] key.*

Accessories

Evolution 300 can be operated with several electrical accessories. The software does not support: Temperature Probe, Rapid Mixing Accessory, 7-Cell Changer in reference beam.

After installing or removing an electrical accessory it is necessary to restart the software so that the new configuration is detected. If the cell changer is not detected, it might be that the instrument is configured such that the cell changer is not active.

The Evolution 300 can be equipped with an automatic sample aspiration system (sipper) that includes a peristaltic pump and a flow-through cell. Sippers can increases sample throughput by automated sample aspiration.

The instrument can be run with Peltier accessory PCCU1, see below.

The sipper sampling volume must be calibrated: see *Manual Control Command* 5-13.

Error Messages

Initialization
When starting the software during initialization, the following error message is displayed:

Instrument is initializing please wait

In this time, the instrument performs a number of internal checks and initializations.

Specific Parameters

The instruments allow a number of specific settings:

- **Integration Time**
  For measurements at fixed wavelengths (Rate, Fixed and Quant applications) an integration time can be entered. This entry determines the time over which the signal is averaged to improve its signal-to-noise ratio. High integration times however increase the measurement time.

- **Lamp**
  The pulsed Xe-lamp automatically is switched off in a stand-by mode, see below. Then the live display shows *******. The lamp immediately resumes operation, if a measurement is initiated.

- **Scan Speed**
  Scan speeds can be selected up to 3800 nm/min. If a fast scan speed has been selected together with a smaller data interval, an appropriate slower scan speed is used automatically.
  A scan speed of 0 nm/min can also be selected. This setting corresponds to the *IntelliScan* mode, where the scan speed is automatically optimized to maintain a constant signal/noise ratio. See: *Spectrometer Parameter Group* 5-15

- **Slit** (Spectral bandpass)
  The Evolution 300 feature a selectable spectral bandpass. The **Slit** setting can be entered in the **Advanced Parameters** window.

Automatic Source Switch-off

The configuration file allows a time for source switch-off to be defined. When the defined time has elapsed after a measurement, the lamp is switched off automatically. This is to limit lamp working hours and so to extend lamp life. See: *Configuration file* 8-3.

Peltier Accessories for Temperature Control

The Peltier Accessory (Air-Cooled) SPG 1A (Temperatur Controller) is an option for the GENESYS 10S platform. It is used for thermostatting rectangular 10 mm cells in the range of 20-60 °C for a measurement.

The Evolution™ Peltier Thermostatting Accessory is a Peltier thermostatted water bath to control the cell temperature with an Evolution 200/300 series spectrophotometer. The accessory can be operated in the range of 0-110 °C, or 5-100 °C (cell changer).

To correctly connect the accessory to the PC, make sure that the port designated *USB Serial Port* is selected in the software. See *Preferences* 5-10 command.

Control of the unit is identical for both versions. When the unit is powered, it automatically enters the **Standby** operation mode. For the control via PC, press the **ON** button to start its operation mode. Hold the button for up to a second. You may preselect an operating temperature on the unit's panel.

Software control of the unit within a method is activated in the **Accessory** window. See *Accessory window* 5-20.

Operation Hints

Control of the temperature is initiated, when a method with activated temperature control is started. The software does not check the cell holder's temperature for the initial baseline correction run; a temperature check however is done for subsequent sample measurements: A sample measurement is delayed until the cell holder reaches the target temperature (+/- selected tolerance).

Tip: *Control of the temperature is not initiated, if the baseline correction run is started via the* ***Baseline/Autozero*** *button of the tool bar.*

Tip: *Control of the temperature can selectively be initiated by starting a method with an appropriate temperature setting and cancelling it immediately. Alternatively, the temperature may also be set at the accessory's panel.*

Tip: *Stirring the sample should be employed to ensure fast and uniform temperature equilibration. For that a small magnetic stirring bar must be inserted to the cell and a* ***Stirring speed*** *must be selected.*

Due to different procedures, the temperature values displayed at the accessory and those transferred to the PC and displayed by the software may vary slightly.

It should be regarded however that the cell contents can have a substantial temperature lag during heating and may also have a permanent temperature difference to the target temperature. For an accurate temperature control of a sample, the effective sample temperature should be checked with a calibrated temperature probe.

Problem Solving

An error message *Error accessing Communications port COM ? (SPG)* is issued by the software, if the accessory's communication protocol is not configured correctly. For software control, the MODBUS protocol must be activated.

To change the configuration, proceed as follows:

1. In operation mode (see above), press the **Menu** button and select the **Configure** item via the **Scroll**/**Select** buttons.

2. Enter [11111] as a password: change the number with the ∧ (up arrow) button and go to the next number with the **Scroll** button. After the last number push the **Scroll** button again.

3. Use the **Scroll**/**Select** button to select the **Communication protocol** item.

4. Select number [6] that correspond to the MODBUS protocol and press **Exit** to return to the operation level.

In some configurations, the above error message persists, if the accessory is attached via a COM port with a number >9. When the system automatically has selected such an inadequate port number, the COM port may be forced to a another COM port number via the Windows Device Manager: From the **Control Panel** open the **Device Manager**; in the **Ports** section right click **Port n USB-Serial Port**; click **Properties**/**Port Settings** tab/**Advanced** button, **COM Port Number** selection. Select a *COM port <10* that is currently definitely not in use. However it may be reserved by Windows for other devices currently disconnected. Ignore the possible warning message, if the port number is reserved by Windows. It is required to reboot the PC to establish

the modification.

10.2 Accessories

Several options are available to implement automated sample aspiration and cell temperature control.

Sipper Accessory

With an automated sipper accessory it is possible to substantially increase the sample throughput of liquid samples. For instruments that do not allows to attach a sipper accessory, a PC-controlled external sipper pump (Economy Sipper) is available, see below.

Note: *The function **Sample return** is not supported with the measurement procedure.*

Note: *When the instrument is equipped with a sipper and a cell changer, the sipper operation is applied.*

In the **Spectrometer** parameter group the software offers an **Accessory** button. Click on this button to open the **Accessory** window, where you enter the sipper parameters. The settings are saved with the method. See: *Accessory Button* 5-18

- The **Sampling time** [seconds] determines the amount of sample that is aspirated. The user has to make sure that the desired volume is sampled with the selected time. Some models use the parameter **Volume** instead. The aspiration **Volume** must be calibrated, see below.

Note: *Make sure that the sampled volume is high enough to fill the flow-through cell and to avoid sample carry-over.*

- The **Wait time** is a short time interval between sampling and measurement to allow the flow to settle and bubbles to rise.

- The parameter **Air gap** defines the option, to aspirate an air bubble after the sample. This separates the sample sections and should improve the cleaning of the tubing. When using this option, the system gives a sound after sampling. The user should remove the sample from the sipper tube immediately. After 2 seconds the sipper is restarted to aspirate air.

Note: *Make sure that this volume is small enough so that the air segment does not reach the flow cell.*

In routine operation, the button at the sipper is applied to start the measurement. Then, the sample is aspirated under the defined conditions, the **Wait time** is run down and then the measurement is started automatically. Alternatively, also the **Sip & Measure** button of the **Sample information** window is applicable.

Alternately you may use the **Sip** button in the the **Sample information** window. Aspirate the sample as long as required. Then use the **Measure** button to immediately start the measurement.

Via the **Manual Control** command in the **Options** menu, the sipper can pump in both directions (sample delivery and return; if supported). To stop pumping click on the red **Stop** button.

The additional function **Calibrate** allows calibrating the aspiration **Volume** for specific Thermo Scientific spectrometers:

Sipper Volume Calibration (dedicated Thermo Scientific spectrometers)

With a first installation, change of solvent and degradation or complete replacement of the pump tubing, the sipper aspiration volume has to be calibrated for specific models:

1. Open the **Options** menu and select the **Manual Control** command. See: *Manual Control* 5-13

2. Within the **Manual Control** window select the **Calibrate** function.

3. Enter the **Volume** to be aspirated for a single cycle.

4. Provide the solvent in a graduated cylinder and enter the desired volume. Initiate the sample aspiration several times with the **Aspirate** button.
   The system will use a corresponding aspiration time, which is based on the existing sipper volume calibration factor.

5. After pressing **OK** enter the actually aspirated total volume.
   The new sipper volume calibration factor is calculated and transferred to the spectrometer.

PC-controlled Sipper Pump (Economy Sipper)

As an alternative to an instrument's sipper accessory an external PC-controlled sipper pump can be applied.

The software supports control of an external peristaltic pump as a sample aspiration system (sipper) via a USB interconnect unit (an electronic relay) that is connected to one of the PC's USB ports. The interconnect unit must be attached to the computer before the software is started in order for it to be recognized by the software.

The software shows the control options for the sipper only when the interconnect unit is attached. Operation details are equivalent to those of a sipper accessory, see above.

Tip: *The USB interconnect unit can also be employed for other purposes that require on/off switching.*

Thermo Scientific Pump Kits

Thermo Scientific offers a selection of peristaltic pumps and Economy Sipper Kits configured for use with different spectrophotometers and with plugs suitable for different regions of the world. Contact your Thermo Scientific distributor for details and specific ordering information.

A kit will typically contain:

- Thermo Scientific single channel peristaltic pump with adjustable flow rate
- Appropriate power cord
- 10 mm flow cell (glass or quartz, as ordered)
- Accessory door and sipper spout for the spectrophotometer, if required
- Silicone No. 16 pump tubing
- PTFE tubing to route through spout

The sipper pump can also support a range of alternative pump tubing sizes and materials to

allow handling of specialized solvents and/or larger or smaller flow rates.

To connect the pump to the PC a USB interconnect unit is available.

Installation of Pump Kit and Interconnect Unit

This section describes the installation of the above pump kit together with a USB interconnect unit. Proceed accordingly for other sets.

1. Install the parts of the sipper kit and tubing according to the directions supplied with the kit.

Tip: *Normally the pump is installed after the flow cell (in the direction of flow) to minimize the volume of the aspiration section. A waste container should be made available at the end of the pump circuit.*

Model Thermo Scientific 9000-1754 sipper pump (reverse side) with interconnect unit attached

2. At the pump, remove the short-circuit contact on the bottom two screws of the connection strip on the back of the unit (connections External Control), and attach the cables from the interconnect unit, one under each screw. Either cable can go under either screw.

Tip: *The pump's Prime start/stop pushbutton is deactivated when the pump is under external control. If an additional manual control switch is required, it can be connected at the same contacts in parallel with the interconnect unit.*

3. Connect the USB connector of the interconnect unit to one of the PC's USB ports. The port configures automatically.

4. Use the lower switch on the pump's front panel to select the appropriate pump direction.

5. With the speed control knob, adjust the flow rate so that a typical pump time of 5-10 seconds delivers a volume that optimizes sample consumption and sample carry-over.

Important:

The software fixes the pump time. Make sure not to change the pump speed thereafter. Otherwise the pump might empty the sample tube and deliver air into the tubing system or might deliver too little sample volume so that the sample does not reach the flow cell for measurement.

Please note that pump tubing is a consumable that must be replaced regularly. The replacement interval will depend on the liquid being pumped, the number of hours of use the pump sees each day and on other factors.

Peltier Accessories for Temperature Control

The Peltier Accessory (Air-Cooled) SPG 1A (Temperatur Controller) is an option for the GENESYS 10S platform. It is used for thermostatting rectangular 10 mm cells in the range of 20-60 °C for a measurement.

The Evolution™ Peltier Thermostatting Accessory is a Peltier thermostatted water bath to control the cell temperature with an Evolution 200/300 series spectrophotometer. The accessory can be operated in the range of 0-110 °C, or 5-100 °C (cell changer).

To correctly connect the accessory to the PC, make sure that the port designated *USB Serial Port* is selected in the software. See *Preferences* 5-10 command.

Control of the unit is identical for both versions. When the unit is powered, it automatically enters the **Standby** operation mode. For the control via PC, press the **ON** button to start its operation mode. Hold the button for up to a second. You may preselect an operating temperature on the unit's panel.

Software control of the unit within a method is activated in the **Accessory** window. See *Accessory window* 5-20.

Control of the temperature is initiated, when a method with activated temperature control is started. The software does not check the cell holder's temperature for the initial baseline correction run; a temperature check however is done for subsequent sample measurements: A sample measurement is delayed until the cell holder reaches the target temperature (+/- selected tolerance).

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2. Enter [11111] as a password: change the number with the ∧ (up arrow) button and go to the next number with the **Scroll** button. After the last number push the **Scroll** button again.

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4. Select number [6] that correspond to the MODBUS protocol and press **Exit** to return to the operation level.

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