

Version 2.51

Scantraq

**Spectrophotometer Software
for Microsoft Windows**

Advanced Measurement Technology from



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User Guide

Getting Started

Scantraq acquires data from *PerkinElmer*, *Agilent (HP)*, *Varian* and *Hitachi* spectrophotometers (see “Input Device” on page 15). The following program files support the listed instruments:

mhp8453.exe	Agilent (HP) 8453
mpe983.exe	PE Lambda 2-45, 9, 650-950 (no URA), 580B - 983G PE Lambda 18/19 Win 98 (PE ISA board)
mpe19AX.exe	PE Lambda 18/19 Win 2000/XP (Lambda AX board)
mpe950.exe	PE Lambda 650-950 (URA)
mpe1050.exe	PE Lambda 1050 (URA/TDM)
mcary5.exe	Varian Cary 1/100-5/5000
mh3410.exe	Hitachi U-3210/3410 (3200/3400)

Mpe983.exe also supports SummaSketch digitizer tablets. This makes it possible to create data files from spectral strip-charts. In addition, Mpe983.exe controls and acquires data from OOI, StellarNet and Zeiss spectrometers via ActiveX servers. Through its built-in programming modules and ability to communicate with other Windows software, Scantraq can be utilized as a component within an automated quality control system. Finally, Scantraq provides means to control several instruments with the same software.

Installation

If the CD-ROM does not autostart, run **..install\setup32.exe** from Start... Run. An installation password and Administrator privileges are required. Setup will not overwrite previous data files.

Scantraq for Cary spectrophotometers requires that Varian's WinUV scan software is installed. Be sure to close WinUV before running Scantraq.

Scantraq for PE Lambda 650-1050 using mpe950.exe or mpe1050.exe requires that PE's UV WinLab is installed. When not using the URA (Universal Reflectance Accessory), Lambda 650-950 can be controlled by mpe983.exe. Close UV WinLab before running mpe950.exe or mpe1050.exe.

Scantraq for PE Lambda 18/19 using mpe19AX.exe requires the Lambda AX PCI parallel card and dual LPT cable which are available from FTG Software.

Complete installation as well as update files can be found at

<http://ftgsoftware.com/updates.htm>

We suggest that you visit this page often to keep your software up-to-date.

Scantraq is initially configured with Test Mode ON. Turn this mode OFF (see “Test Mode” on page 9) before attempting to acquire data.

A Security ID Module must be attached to the parallel or USB port. Please report any problems when installing or running Scantraq. Contact information is provided in **Help...About**.

When installing with USB Security ID Module for the first time, DO NOT plug in the module until installation is completed! Windows will automatically locate the new device.

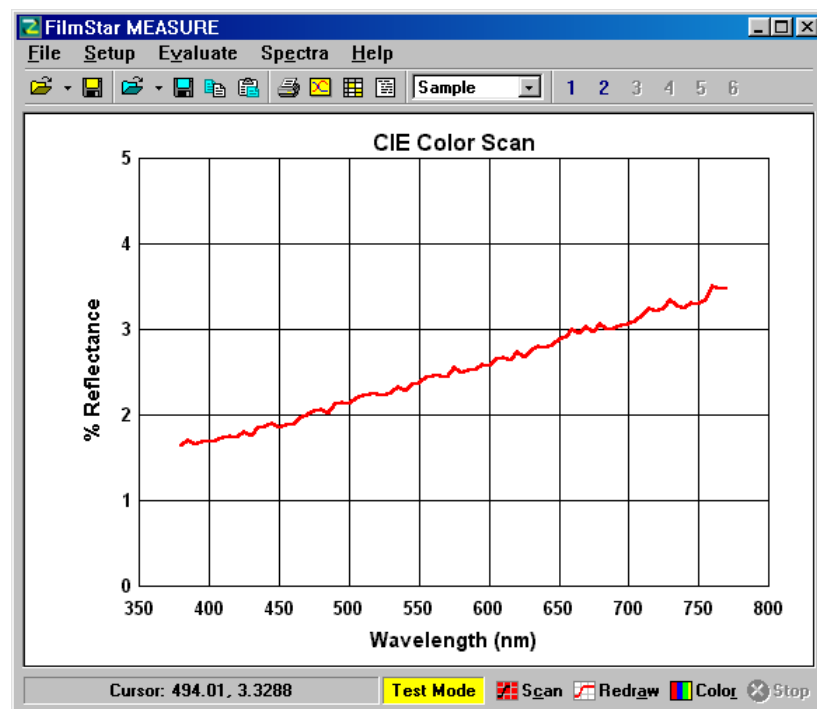
Scantraq provides an extensive set of Help screens. Press <F1> from any menu item or dialog box for context-sensitive help. The help system is identical to this manual's Reference section.

Tutorial

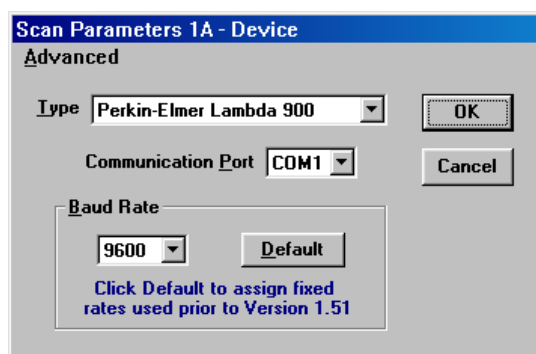
Scan Method

Double-click the Scantraq icon. The screen shown below appears. If label **Test Mode** is not displayed, click **File...Configuration...Preferences** and check the box labeled **Spectrophotometer Test Mode**.

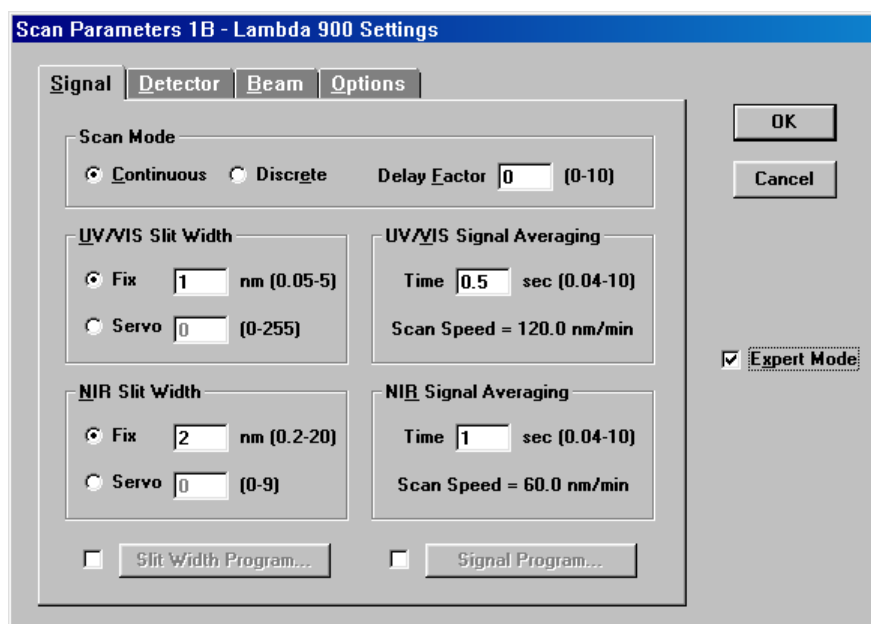
Please remember to disable Test Mode when actually acquiring data from your spectrophotometer!



We start by examining the Scan Method (see “Instrument Settings” on page 18) which are edited in linked dialog boxes. Click **Setup...Scan Method <Ctrl+M>**. a Scan Method includes instrument settings, graph ranges, etc. As shown below, Screen 1A selects the **Input Device** which can be a spectrophotometer, digitizer (rarely utilized), or server (raw or processed data).



At this point click **OK <Enter>** to accept any changes in the dialog box or click **Cancel <Escape>** to undo any changes. Either key brings you to the next Scan Method screen - **Instrument Settings**. (To quit Scan Method setup and return to the Main Menu, click **Cancel** as each dialog box appears or type **<Alt+F4>** to exit the sequence.)



Since choices depend on the particular spectrophotometer, the instrument's manual should be consulted for information about particular settings.

Scantraq supports two **Scan Type** modes:

1. **Continuous**...This is an spectrophotometer's native scan mode, equivalent to pressing the instrument's scan button. A scan range is defined and the instrument slews smoothly from initial to final wavelengths.
2. **Discrete**... The instrument slews to a wavelength, stops, reads transmission values, and proceeds to the next wavelength, etc. Scan ranges may include inverse wavelength spacing or custom lists. Accuracy can be increased with a **Delay Factor**. This causes the instrument to wait

$$t = (\text{Delay Factor}) * (\text{Filter Response}) \text{ seconds}$$

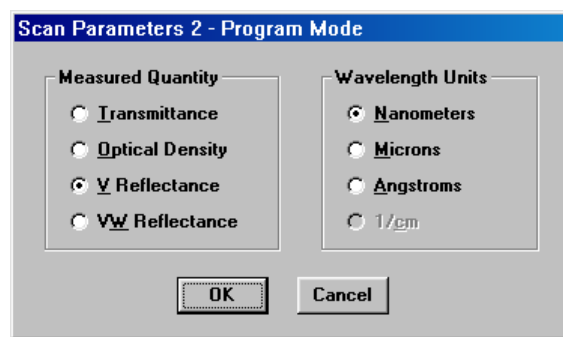
before reading data. Delay Factor is not required in newer instruments using digital technology.

When measuring narrow filters it is might be useful to scan bandpass zones with fine wavelength intervals (*i.e.* 1 nm), and blocking zones with coarse intervals (*i.e.* 10 nm). This ensures accuracy with optimum measurement throughput.

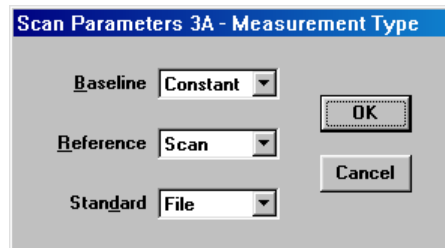
The superiority of one or the other Scan Type mode depends on the particular requirements of the spectrum being measured as well as the characteristics of the spectrophotometer in the spectral region.

Users should convince themselves that a selected scan speed accurately delineates spectral features. Try a test run with a slower speed to see if there are significant differences.

Moving onward by clicking OK or Cancel we arrive at the **Program Mode** screen shown below. Whether one or all **Wavelength Units** are enabled for selection depends on whether Continuous or Discrete scans were selected in the previous screen. The two reflectance modes are discussed in “Data Type” on page 13.



The next screen defines **Measurement Type** for Baseline, Reference and Standard data files. Since there is often no need for Baseline scans with modern instruments, we enter *Constant* next to **Baseline**. (The actual value is assigned later.)

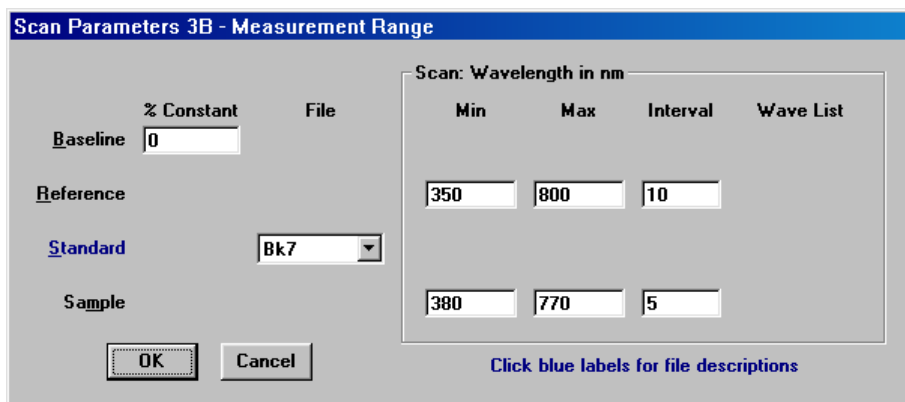


We plan to measure the reflectance of AR coatings on BK7 substrates over the CIE color range 380-780 nm. Since previous experience indicates that best accuracy is obtained if we scan an uncoated substrate (ground second surface) at the start of each measurement series, we enter *Scan* next to **Reference**.

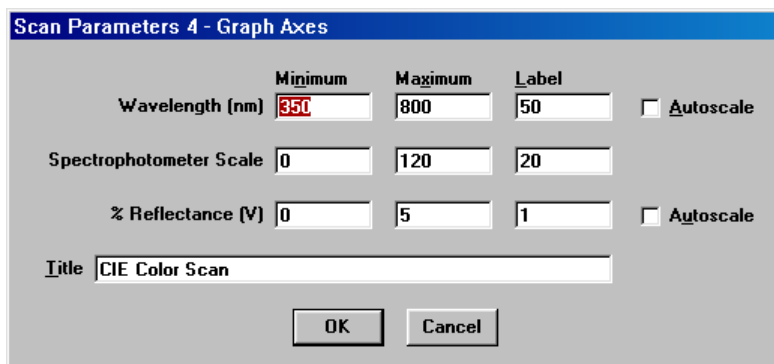
The Reference scan will provide spectrophotometer readings for our BK7 substrate. But what does that really correspond to? Fortunately we have a disk file containing actual BK7 reflectance values as a function of wavelength. In order to use this file we enter *File* next to **Standard**.

Click **OK** or **Cancel** to proceed to the next screen - Measurement Range. The active data entry fields depend on selections made in the previous screen. For example, if you really want to enter Constant = 4.2% for **Standard** instead of file "bk7", you must return to the Main Menu and re-edit the Scan Method.

There are no data entry boxes under **Wave List**, because Continuous rather than Discrete scan mode was specified. A wave list refers to an existing list of wavelengths. For more information see “Wavelength List” on page 21.



The above dialog can be accessed directly from the Main Menu by clicking **Setup...Measurement Range <Ctrl+A>**. Press OK or Cancel once more for the final Scan Method screen - Graph Axes.



Range and Axes can be edited by without looping through the entire Scan Method.

This dialog can be accessed from the Main Menu by clicking **Setup...Graph Axes <Ctrl+G>**. Note that Scantraq displays different graphs during and after the scan. While scanning the graph monitors actual values sent by the spectrophotometer. Here the vertical scale is set by **Spectrophotometer Scale** settings. This scale is also used for Baseline and Reference readings.

Upon scan completion Sample data is corrected for Baseline, Reference and Standard data arrays. The corrected data is plotted on a user-defined scale, in this case **% Reflectance**.

Test Scan

Place the instrument in Test Mode (*Test Mode* displayed in status bar), click **File...Open <Ctrl+F12>** and load an appropriate Scan Method: "pe2.scw" (use for PE Lambda 2-45), "pe9.scw" or "pe983.scw", etc. These files set Scantraq for %T readings where Baseline = 0%, Reference = 100% and Standard = 100%.

All ".scw" files are not the same. Do not load a Scan Method that is inappropriate for your spectrophotometer or version of Scantraq. If controlling more than one instrument with the same computer, use different directories.

Click **Scan <Alt+C>**. The Test Mode trace is a straight line.

Disable **Test Mode** in **File...Configuration...Preferences**. We're ready to see if Scantraq really works with your instrument. Click **Setup...Initialize <Ctrl+I>** (if available) to issue initialization commands. Normally you are prompted for initialization after loading a new Scan Method. Since we've just switched from Test Mode we issue the command manually to test it.

Depending on instrument, the status bar at the lower left might now display "Initializing - please wait" for a few seconds. Depending on instrument, a series of messages provides feedback that things are working properly. If there is a communications error Scantraq ultimately issues an appropriate message.

If that happens, there are several possibilities:

1. Is the correct cable installed? If a RS-232 modem cable doesn't work try a null-modem cable or adapter. Lambda 2 and similar older models require a custom 25 pin to 9 pin connector (contact PE).
2. Was the correct COM port or GPIB device specified in the Scan Method?
3. Does the serial configuration match those expected by Scantraq?
4. Lambda 950-1050 with URA (universal reflectance attachment) or TDM (triple detector module) requires UV WinLab. Do not run Scantraq and UV WinLab simultaneously.
5. Cary operation requires Win UV installation. Do not run Scantraq and Win UV simultaneously.
6. Lambda 18/19 (Windows 98, SQPlot) is supported by Mpe983.exe with 16-bit L19Svr.exe which must be activated before Scantraq can communicate with the instrument.
7. Lambda 18/19 (Windows 2000/XP) requires a computer with built-in LPT (parallel port). A Lambda AX board adds a second LPT port.

For further details, see "Input Device" on page 15.

Remove any optic or reflectance attachment from the sample chamber.

Click **Scan <Alt+C>** and listen for the sound of your instrument's scanning motor. The graph will update as data is acquired. If you don't see a trace click **Spectra...Data Table** to view the data in tabular form. Possibly data are out-of-range for the graph axes.

If the spectrum is not flat at T=100%, it can be corrected with a Reference scan. Click **Setup...Scan Method <Ctrl+M>** and set **Reference** to **Scan** in Screen 3A (Measurement Type). In Screen 3B (Measurement Range), enter **Reference Min**, **Max** and **Interval** values. Note that **Standard** remains equal to 100%.

Upon returning to the Main Menu, place Scantraq in Reference mode with **Setup...Data Type...Reference <Ctrl+R>**. Click **Scan <Alt+C>** to acquire data. At the conclusion of the Reference scan, return to Sample mode and scan again. Is the spectrum now flat at 100%T? Finally, place an optic in the sample chamber and measure its transmission.

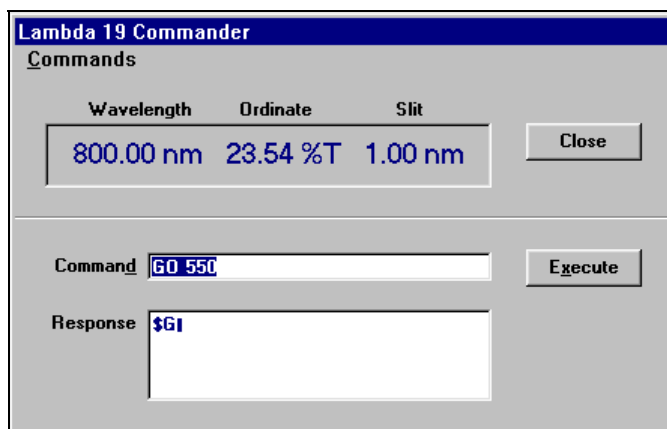
Spectrophotometer Commands

Setup...Commands <F2>

The Lambda 19 can be operated in simulation mode (Windows 95/98 only) by substituting "lamsim.exe" for "lamcon2.exe" in "autoexec.bat". Be sure to turn Scantraq Test Mode off.

Since a number of instruments can only be operated from a computer, we include **Commander** screens as illustrated below. The **Wavelength-Ordinate-Slit** live display text box is automatically updated several times each second.

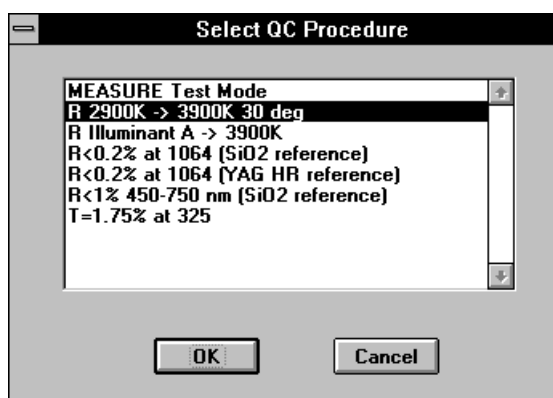
Type a command *without the leading '\$' character* in the **Command** box and click **Execute**. Click **Commands** for a pull-down menu with useful commands. Click **Commands...Scan Method <Ctrl+M>** to access Instrument Settings (Scan Method screens 1A and 1B).



Automating Scanraq

While most users will (at first) think of Scanraq as a standalone program, it can also be used as a component within a larger Windows applications. A typical example is quality control. Spectra must be measured and interpreted according to specific criteria such as CIE color or bandwidth. Documentation including spectral curves may be required. The user might also want to store results on disk and update a database with relevant information.

The application can also isolate technicians from the complexities of instrument and software setup. In the example illustrated below, the technician inserts an optic in the sample chamber, selects a QC Procedure and clicks **OK**.



Reference

File Menu

Open <Ctrl+F12>, Save <Shift+F12>, Save As <F12>

The Scan Method file (name displayed in Windows title box) is opened and saved in the File Menu. Wavelength List files are accessed in the Setup menu and spectral data files through the Spectra menu.

Copy Graphics

Copies the current screen graphic to the clipboard for pasting into other applications.

Print Graphics <Shift+Ctrl+F12>

Print the screen graphic to the current Windows default printer. Best results are obtained with a white background.

Exit <Alt+F4>

Upon exiting configuration file "..\Scantraq\config\scantraq.ini" is updated. The current Scan Method is automatically saved in file "work.scw".

Configuration - Capacity

File...Configuration...Capacity

Users can configure Scantraq for optimum memory utilization by entering values which do not exceed anticipated maxima. Changes are implemented when Scantraq is exited and restarted. Failure to allocate sufficient space usually leads to a 'Subscript out of range' error.

It is not necessary to scan wavelengths at the same interval for each data type. Baseline, Reference and Standard data will be interpolated at the Sample scan interval. That is, reference data scanned every 10 nm can be used with sample data scanned every 1 nm.

Configuration - Directories

File...Configuration...Directories

Scantraq uses four file extensions for storing and loading different types of data. Files are stored in three default directories. While files can be loaded from any directory, they can only be stored in default directories. (Exception: spectral sample data files can be stored anywhere.)

Data

Scan Method (*.scw) and Wavelength List (*.wls).

Sample

Spectral data files (*.csv) in 'comma-separated values' ASCII format. These files can be loaded as Excel worksheets. Since ".csv" is a standard Excel

extension, users should create unique directories for spectral data files: i.e. "c:\excel\spectra". These files can be loaded directly into Scantraq.

Reference/Baseline/Standard

Data files in ASCII format (Reference/Baseline *.dat, Standard *.csv)

Database Configuration

Scantraq BASIC programs can be assigned to *DB Retrieve* and *DB Save* menu commands in the File and Spectra menus. An example is the FileMaker Pro database solution included with Scantraq. The examples show how database technology and ActiveX provide means to sort and select measured spectra. Users are not restricted to FileMaker Pro. MS Access programmers can develop similar functionality.

Enter file names of BASIC programs to be assigned to menu commands. Click **Edit...Select <F3>** to browse and select files.

Configuration - Preferences

File...Configuration...Preferences

Use Windows message box

Message boxes display **OK Cancel**, **Yes No** and similar messages. You have a choice of Windows default message boxes (screen centered) or FTG Software message boxes (usually centered in active window). Windows message boxes support Windows sound effects. You may find FTG message boxes somewhat easier to read.

Cancel warning

Warning message upon leaving a data entry form with **Cancel**.

Overwrite warning

Warning when opening a new file or saving a file after changes in the data.

Automatic Edit

Edit the Scan Method immediately after loading a new file from disk.

New axes

Automatically draw new axes when Graph Axes parameters are changed. Turn off this feature to superimpose %R and %T plots on the same graph.

Test Mode

Especially useful for developing Scantraq BASIC programs off-line. The words *Test Mode* are displayed in Scantraq's status bar.

Lambda 19 Windows 95/98 users can use simulation software instead of Scantraq's test mode. This is accomplished by substituting "lamsim.exe" for "lamcon2.exe" in "autoexec.bat".

There are occasions, *i.e.* when developing quality-control models, when realistic data are required in Test Mode. This is accomplished by selecting **Test Files...** and specifying a Baseline, Reference and/or Sample file names. Advanced users should note that these file names can also be specified via DDE. These file names are ignored when Test Mode is deactivated.

Display and save file descriptions

Check to save and list file descriptions (50 characters maximum). This facility is a carry-over from 16-bit Windows (8 character file names). The option adds **File...List** and **Spectra...List** commands.

The above preferences are automatically stored upon exiting Scantraq and responding **Yes** to 'Save new configuration'. The following advanced preferences are set by manually editing "..\Scantraq\config\scantraq.ini". Do not type comments (starting with ;) on the same line as a setting. The values shown are usually the default values assigned when any of these lines are not in "scantraq.ini". Lines can be added anywhere in the appropriate section.

CIE User-Illuminants

Users can add any number of illuminant files as follows. For further information see "CIE Color Module" on page 51.

```
[CIE Color]
Illum1=Xenon Lamp;arclamps\xenon.csv
Illum2=Fluorescent Cool;fcool.csv
Illum3=Fluorescent Warm;fwarm.csv
```

The first description appearing in the pull-down illuminant list is *Xenon Lamp* and the corresponding file name is *xenon.csv*. Files should be stored the Scantraq program directory (usually c:\Scantraq), but an optional subdirectory (arclamps) can be added.

Status Label

The status label font at the screen lower left can be changed from bold (default) to normal; text alignment can be changed from center (default) to left or right justification. Enter or edit the following line(s):

```
[Configuration]
StatusLabelBold=-1 ;0=normal font, -1=bold font
StatusLabelAlign=2 ;0=left, 1=right, 2=center justify
```

Scan graph background color

Colors displayed during spectrophotometer scans may be adjusted with the following line(s):

```
[Configuration]
ScanBackColor=12 ;red
ScanAxesColor=7 ;gray
ScanLineColor=0 ;black
```

where

0	Black	8	Dark Gray
1	Dark Blue	9	Blue
2	Dark Green	10	Green
3	Dark Cyan	11	Cyan
4	Dark Red	12	Red
5	Dark Magenta	13	Magenta
6	Dark Yellow	14	Yellow
7	Gray	15	White

Stop button enabled

It is possible to abort a continuous scan by clicking **Stop <Esc>**. Users can enable/disable this and related functions by adjusted the following line(s). 0 is False (no) and -1 is True (yes).

```
[Configuration]
AutoModeStop=0 ;Enable Stop when Auto-Activate ON
```

```
ContinuousScanStop=-1 ;Enable Stop in continuous scan
DiscreteScanWarn=-1 ;Warning after discrete scan Stop
```

Prevent overwriting J-CAMP .dx files loaded from disk

To help minimize the inadvertent corruption of J-CAMP data files loaded from disk, set the following flag. You can still overwrite a file with the same name, but only after a scan is performed.

```
[Files]
NoOverWriteDX=-1
```

PerkinElmer break character

When stopping a continuous scan (PE only), a break character is sent to the spectrophotometer. Normally this is ASCII 35 ('#'), but can be changed if necessary. This adjustment is included because of uncertainty regarding 983 models, and the possibility of changing the break character on the Lambda 2. It should not be changed for Lambda 5/7/9 and has no effect for Lambda 19.

```
[Configuration]
BreakCharacter=35 ;Break character is ASCII 35
```

PerkinElmer startup initialization prompt

When Scantraq first starts the 'Reinitialize' prompt appears for PE Lambda models. The prompt can be suppressed as shown below.

```
[Configuration]
StartUpInit=0 ;No Reinitialize' prompt at startup
```

HP 8453 Buttons

Normally HP 8453 buttons are disabled. This ensures that control is from the computer, especially when running Scantraq BASIC macros. To enable the buttons enter the following line.

```
[HP 8453]
EnableButtons=-1
```

Multiple Instruments

This is only required when two or more spectrophotometers *of the same type* are connected to the same computer *and* Wavelength Calibration is being utilized. When enabled, Instrument 1-4 is selected in the Scan Method 1A Device dialog.

```
[Configuration]
MultiInstruments=-1
```

Configuration - Security

File...Configuration...Security

ID Module

An FTG Software HASP Security ID Module must be attached to the parallel (printer) or USB port. HASP modules are embedded with company name. Users who experience difficulties should visit

<http://www.ftgsoftware.com/issues.htm>

and click *Security ID Module doesn't work* under *Installation & Startup*.

Configuration - Miscellaneous

File...Configuration...Misc

Graph Axes Labels provides the means to replace English graph axes labels with international equivalents. Labels apply to the SQPlot Module as well as the main screen.

Setup Menu

The Setup Menu establishes numerous program conditions. Some selections do not apply to instruments which do not support the particular feature.

Data Type

Select Sample, Baseline, Reference or Standard data files. Baseline and Reference modes are enabled or disabled according to the Scan Method.

Scan Method <Ctrl+M>

Edit instrument parameters in a series of linked screens. The Scan Method is opened and saved in the File Menu.

- 1a Select input device and COM port
- 1b Spectrophotometer settings
- 2 Program mode - plot type and units
- 3a Measurement Type - select Constant/File/Scan for each Data Type
- 3b Measurement Range - specify scan range, file names and/or constants
- 4 Graph Axes - specify graph axes for measured and reduced data

Measurement Range <Ctrl+A>

Instant access to Scan Method Screen 3B.

Graph Axes <Ctrl+G>

Instant access to Scan Method Screen 4.

Wavelength List

Generate a custom wavelength list for acquiring data at specified wavelengths using Discrete scan type (set in Scan Method screen 1b).

Initialize

Execute instrument-dependent commands such as Page 1 (Lambda 9), lamp configuration (Lambda 2/19), slit width (Lambda 2/5/7/9), detector switch wavelength (Lambda 9/19), NIR sensitivity (Lambda 9/19), etc. This command must be executed at startup and whenever instrument parameters have changed.

Spectrum 2000 users should issue this command if the current Spectrum setup (.set) file has been changed by another program.

Calibrate Wavelength

Determine wavelength correction functions from a series of known wavelengths.

Auto Zero (Background Correction)

Perform auto zero and background correction using the spectrophotometer's internal capability. Users must use baseline and/or reference scans for older models which do not support automatic correction.

Lamps ON

Allows Lambda 2/19/900 users to turn lamps off to conserve bulb life. This is a toggle command which is checked when the lamp is on. When turning bulbs back on, be sure to allow sufficient time for stabilization.

Commands <F2>

Send commands directly to a Lambda 19/900. Especially useful for slewing the instrument to a particular wavelength.

Auto Zero and Background Correction

Setup...Auto Zero

Enter the anticipated wavelength range/scan speed. The Scan Speed can usually be greater than the sample scan speed when the spectral response of the reference optic or empty sample compartment is relatively flat. Calibration must be repeated for different sample holders and masks. **Use Scan Range Settings** updates displayed values with the current Scan Method settings.

PE auto zero settings are saved in configuration file
"\\Scantraq\config\scantraq.ini".

Since there is no built-in background correction, Lambda 900 models do not require an auto-zero function. Users should use Scantraq's Reference mode to duplicate this functionality.

Data Type

Setup...Data Type

There are four data types in Scantraq:

Sample

Scan with coated optic mounted in the sample chamber. Measured values are displayed during data acquisition (spectrophotometer units, 0-100% T); Reduced (final) values are displayed upon returning to the Main Menu (physical units 0-100% R/T or Abs). If required, Baseline and Reference scans must precede any Sample scan.

Baseline

'Zero' reading corresponding to scanning when the sample compartment is blocked. Baseline data can be stored on disk and automatically utilized in Sample scans. In modern instruments, baseline measurements are often not needed. This depends, however, on measurement scale. Baseline scans may be required when for very low reflectance sample where background noise (scatter) can be significant.

Reference (PE-2000 Background)

Scan with empty sample compartment or uncoated optic. Reference data can be stored on disk and automatically utilized in Sample scans.

%T or Abs	100% scan (sample removed)
%R (V)	Uncoated scan (uncoated glass, reference reflector, etc.)
%R (VW)	V-path scan
%R (VN)	V-path scan for PE URA (mpe950.exe)

Scan with empty sample compartment or uncoated optic. Reference data can be stored on disk and automatically utilized in Sample scans.

Standard

Independently determined %T or %R values corresponding to the Reference scan. A typical example is the V mode reflectance of an AR coating on glass: Reference data is the measured spectrum of the uncoated glass; Standard data is the known reflectance.

Standard data is not used in VW mode. Data can be edited in Scantraq and stored on disk for automatic utilization in Sample scans.

Reduced Sample values are given by

$$\begin{array}{ll} \%T/Abs/\%R(V) & Y=Ystd*(Ymea-Ybas)/(Yref-Ybas) \\ \%R(VW) & Y=SQRT((Ymea-Ybas)/(Yref-Ybas)) \\ \%R(VN) & Y=(Ymea-Ybas)/(Yref-Ybas) \{PE URA\} \end{array}$$

where Y = Final Sample in user-defined units, Ymea = Measured Sample in instrument %T units, Ybas = Baseline, Yref = Reference, and Ystd = Standard.

As specified in Scan Method screen 3A, constants, data files or scans may be used for Baseline and Reference data. Constants and data files may be used for Standard data which may not be scanned.

There may be no need for Reference scans or Standard data in %T measurements for instruments which have built-in 100% reference correction (sometimes called *Autozero*) ; in such cases specify Reference = 100%. Note that newer instruments do not have built-in 100% correction, relying instead on the controlling software.

The user should convince himself that an instrument's built-in zero or 100% correction is sufficiently accurate and repeatable for the measurements being performed.

If Constants are used for all three data types and have respective values Baseline 0%, Reference=100%, and Standard=100%, measured and reduced values are equal and Sample data is labeled Absolute'.

Calibrate Wavelength

Setup...Calibrate Wavelength

This dialog provides means to set up wavelength correction functions. While such correction functions are probably not required (some instruments have built-in calibration), they are included just-in-case.

Enter 3 to 6 known wavelengths which are as widely spaced as possible over the range of interest. Click **Get Coefficients** to compute a quadratic fitting function and **Test** to test the function.

Correction routines are different depending on whether *Continuous* or *Discrete* scan is specified in the Scan Method. In continuous scanning (the usual mode) measured wavelength arrays contain corrected values. If *Auto-convert Sample* is checked, the Sample spectrum is finally converted to the Scan Range specified in the Scan Method.

In discrete scanning, the instrument slews to the instrument wavelength corresponding to the required value specified in Scan Range. For example, suppose instrument = 550 nm really corresponds to 552 nm. In continuous scanning the instrument measures at 552. Then if *Auto-convert Sample* is checked the value at 550 nm is derived by interpolation. In discrete scanning the instrument is driven to 548 corresponding to an actual value of 550.

Graph Axes

Setup...Graph Axes <Ctrl+G>

During data acquisition the user observes measured transmittance values. When the scan is completed the graph is replaced by another one showing corrected (reduced) data.

Wavelength

The wavelength range need not be the same as the scan range. Try range 350 - 800 x 50 nm when scanning from 380 to 780 nm (CIE color coordinates) for a more pleasing graph.

Spectrophotometer Scale

Actual instrument readings in %T units. It may be necessary to set the minimum < 0 for proper graphing when measuring blocking regions. Setting the maximum > 100% may also be necessary.

Transmittance (Reflectance)

Scale for reduced (compensated for baseline, reference and standard values) data. In addition to the graph title, labels may be placed on the graph by pressing <Shift+Click> when the cursor is in the plot area (crosshair shape).

Autoscale

When scanning, wavelength range is determined from the scan range. After the scan vertical axis range is computed from maximum and minimum spectral values. Autoscale is also performed when opening, pasting or importing data. Turn off Autoscale to display multiple spectra on the same graph, since axes are recalculated and redrawn after each scan.

Input Device

Setup...Scan Method <Ctrl+M> (Screen 1A)

Scantraq uses the following RS-232 default serial port settings:

SummaSketch Tablet	9600,0,8,1
PE Lambda 2..45	4800,N,8,1
PE Lambda 5/7/9, 983G	4800,E,7,1
PE Lambda 900	9600,N,8,1
PE 983	9600,E,7,1
PE 881/882/883	9600,N,8,1
Hitachi U-3210/3410	4800,E,7,2

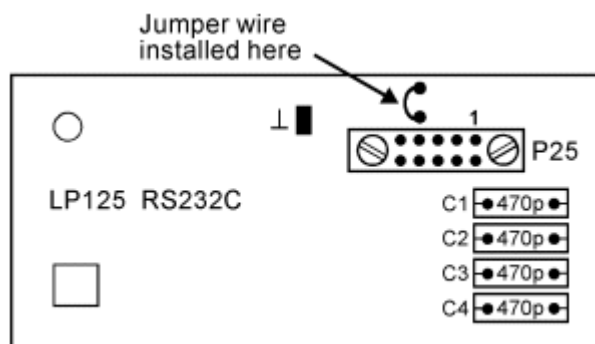
The difference between SummaSketch and SummaSketch II is that Scantraq can automatically set the newer model to ASCII output format. Users with the older tablet may need to open the instrument and adjust a jumper wire.

Click **Advanced** to enable serial CD (carrier detect) and/or CTS (clear to send) error checking or to disable timeout errors. By enabling CD or CTS (we are not sure which works on which spectrophotometer) the program will give instant notification of communication errors rather than wait for timeout errors (5 sec minimum but could be minutes). Disabling timeout errors may be required if your computer cannot handle multitasking.

Special Notes:

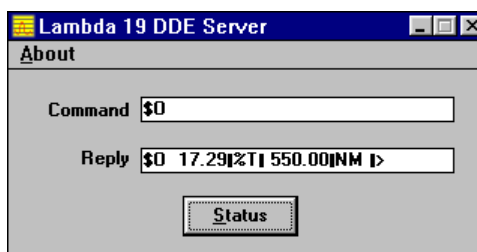
1. **PE Lambda 5/7/9:** If your instrument was originally delivered with a PE Data Station (pre-IBM PC era) you should modify the LP125 RS-232

interface board by installing a jumper wire as shown in the following diagram taken from PE Service Data Bulletin 9-6, 30 June 1987:



For further information on this modification please contact the PerkinElmer service department.

- 2a. **PE Lambda 19 (Win 98):** This instrument is connected to a PE interface board under control of Lamcon2.exe. Since 32-bit programs cannot call 16-bit dll's, 16-bit FTG-developed DDE server L19svr.exe sends messages to and from 32-bit Scantraq. Start the server L19Svr.exe before running Scantraq.



Win 95/98: Lamcon2.exe is run by autoexec.bat at startup. The typical autoexec.bat command line is given below:

```
LH C:\Winfilm\Lamcmd\Lamcon2.exe /350/7/519
```

For simulation, Lamcon2.exe can be replaced with Lamsim.exe. "/7/" in the above command refers to jumper setting on the Lambda 19 board. Use 510 for Lambda 19 UV/Vis and 518 for Lambda 18.

- 2b. **PE Lambda 19 (Win 2000/XP):** This solution is supported on computers with built-in LPT port. A PCI board adds LPT2. A custom cable combines the two ports into a 37 pin Lambda connector. Contact FTG Software to purchase the board.

NOTE: If the following is outside your comfort zone please contact FTG Software or your IT department for assistance.

Installation of LPT2 is not automatic. Run the Control Panel Add Hardware wizard and (after installing Scantraq for Lambda 18/19) locate the following installation file (copied to your hard disk during Scantraq setup) in response to 'Have Disk'.

```
c:\Winfilm\TVicLPT\SETUP_NT.INF
```

Several wizard passes are necessary for complete installation. When the wizards are finally done, locate the above INF file in Windows Explorer, right click on it and then click Install.

In Control Panel select System and click the Hardware Tab followed by Device Manager.

- a. Right click on PCI Parallel Port, select Properties, and access Port Settings; set LPT Port Number to LPT2 (it will probably indicate LPT3) and *Filter Resource Method* to 'Never use an interrupt'.
- b. Right click on LPT1 and change Port Settings *Filter Resource Method* to 'Use any interrupt assigned to the port'; also check that Resources IRQ is set to 07 (normally is).

[Click here for further information.](#)

- 2c. **PE Lambda 2/10/12/14 etc:** The 25-pin male connector can be configured as printer or computer port in *SuperUser* mode. A custom cable may be required.
3. **H-P 8453 Diode Array:** The GPIB (HPIB, IEEE-488) card is used. There are various configurations as indicated below. Configuration is specified in `..\winfilm\config\measure.ini` before starting Scantraq. If you have problems, please contact FTG Software.
 - a. National Instruments cards (ISA/PCI/PCMCIA). You should not need to change default properties. We suggest you reset the HP 8453 address to 8 (dipswitch settings 00001000). This corresponds to the default *GPIB Device Name* DEV8 in Scan Method screen 1A (Input Device).

[HP 8453]
IEEE488=NI488 , GPIBO
 - c. Agilent HP-IB boards require Agilent's Standard Instrument Control Library (SICL). Enter the 8453's HP-IB address in *HP-IB Device Address* in Scan Method screen 1A (Input Device). While it is not necessary for ChemStation to be installed, it may be advisable as Agilent technicians will not be familiar with Scantraq.

[HP 8453]
IEEE488=HPSICL , Hpi b7
4. **Varian Cary 1/100-5/500, etc.:** Scantraq communicates via `cary32.dll`. This required system file is installed by Varian's WinUV package. Note that WinUV must be closed while running Scantraq.
5. **ActiveX Server:** This 'device', included in the PE version of Scantraq, enables communication with ActiveX EXE servers controlling diode-array and FTIR spectrometers. Since the servers can be utilized by other software, baseline and reference calculations are performed in the server rather than in Scantraq. The server returns a corrected spectrum.

ActiveX servers are controlled by Scantraq macros. For ease-of-use, macro commands can be assigned to commands in the Setup menu and to the Scan button.

6. **Hitachi U-3210/3410 (3200/3400):** Parameters such as scan speed and wavelength range are not set individually. Instead, they are bundled and stored in instrument Menu 1-20. Scantraq provides means to load from disk, download from the U-3410, upload to the U-3410, edit, and save parameters on disk.

Note that the Hitachi Measurement Range screen includes an additional Menu Number column where the user specifies which parameters will be used during Baseline, Reference and Sample scans.

Before scanning, the user should ensure that the parameters stored in the Hitachi U-3210/3410 correspond to Menu Numbers specified in the Measurement Range dialog. Scanning may alter previous values stored in Hitachi Menus. Please refer to Hitachi documentation for descriptions of parameter settings.

7. **PE Lambda 650-1050 using mpe950.exe or mpe1050.exe:** *UV WinLab* library MSLambdaServer.exe connects the instrument to Scantraq. If there are errors when Scantraq connects to the server, it is likely that MSLambdaServer.exe was not terminated properly. Use <Alt-Ctrl-Del> to bring up the Windows Task Manager and then delete MSLambdaServer from the Processes list. Alternatively, reboot your computer.

Instrument Settings

Setup...Scan Method <Ctrl+M> (Screen 1B)

Scantraq supports two Scan Mode types:

Continuous

Normal built-in scan method. Scans are usually specified in the instruments 'native' units. In IR instruments (1/cm native units), scans may also be specified in nanometers and microns. Here the actual scan is in 1/cm and final results are interpolated.

Discrete

Special Scantraq scan method. Scan may be specified in any wavelength unit. Wavelength Lists and scan intervals Interval < 0 (closer spacing at short wavelengths) are supported.

In Discrete Mode the instrument slews to the next wavelength and acquires data. A **Delay Factor** may be specified. After slewing to the next wavelength, the instrument waits Delay Factor times **Filter Response** before starting the measurement. This mode is not supported in FTIR instruments.

Note the following instrument-dependent settings and characteristics:

1. **PE Lambda 2**...Slits are fixed at 2 nm; 'Smoothing' simulates variable slit width electronically.
2. **PE Lambda 5/7/9**...Enter 'W' for fixed slit width and 'G' for fixed gain.
3. **PE Lambda 19**...Includes an Integration Time setting and does not require a Delay Factor setting.
4. **PE 88x/983G**...Delay Factor is actual delay in seconds. Noise Filter=0 (.5 on the VDU) is not allowed for Scan Modes=5 to 7. If this rule is violated an error occurs at the beginning of the scan.

ActiveX Commands

This dialog appears when *ActiveX Server* is selected as input device. In this mode data acquisition and normalization (reference correction, etc.) are performed in an external server. As servers can be utilized by other Windows programs, this is different from devices actually controlled by Scantraq.

Servers are accessed and controlled through Scantraq BASIC macros. Entering file names enables Setup menu entries for Initialize, Dark, and Reference scans; the Scantraq Scan button is assigned to the Sample Scan entry. Use **Edit Select <F3>** to browse for BASIC file names.

Device Name lets you replace the default name *ActiveX Server* with a more appropriate device name which appears in status boxes and, most importantly, in the *SPECTROMETER* entry in J-CAMP (.dx) files.

Spectrophotometer Commands

Setup...Commands <F2>

1. **Lambda 19/900**...Send various direct commands. Type the command (without leading character '\$') and click **Execute**. A list of commands can be obtained from PerkinElmer. Some commands have been programmed and are accessed with **Commands**. Select **Scan Method <Ctrl+M>** to adjust instrument settings.

Most erroneous commands return an error message while others do not. In the latter case the command starts with letter 'g' and the Lambda 19 interprets it as go to zero nanometers.

Commands can be tested off-line when "lamsim.exe" is substituted for "lamcon.exe" in "autoexec.bat". The spectrum that is obtained resembles the one in Scantraq's own test mode.

Measurement Range

Setup...Scan Method <Ctrl+M> (Screen 3B)

The contents of this screen depend on selections in the previous **Measurement Type** screen (Scan Method screen 3A) where the type of data (Constant, File, and Scan) is specified for Baseline, Reference and Standard modes.

Constant

Enter a constant value in %. For transmission measurements with modern self-correcting spectrophotometers, Baseline = 0%, Reference = 100% and Standard = 100% are typical. If you are not satisfied with the instrument's built-in 100% correction, the Reference should be scanned.

For 'V' reflection with a glass substrate typical values are Baseline = 0% and Standard = 4.2%. Reference data must be scanned or loaded from disk.

File

Type the name of a previously stored data file. This file will be automatically loaded and utilized during data acquisition. For example, Standard Constant = 4.2% could be replaced with File BK7.

Scan

Enter numerical values corresponding to continuous or discrete scan modes.

Note the following for particular instruments:

1. **SummaSketch**...Sample scan values are utilized in **Spectra...Convert Table**. This allows digitizer scans to be converted to regularly spaced wavelength intervals or lists. Otherwise, scan ranges are ignored when using the digitizer.
2. **PE Lambda**...In continuous scan mode intervals larger than 1 nm must be integers. For example, 2.5 nm is not allowed.
3. **680/780/88x/983/983G**...In continuous scan mode intervals larger than 1 cm⁻¹ must be integers. For example, 2.5 cm⁻¹ is not allowed. When scanning in nm or μm the actual data is collected in cm⁻¹ with the final array calculated by interpolation.

Discrete scan mode is more flexible and possibly more accurate. Depending on settings, it can be faster or slower than continuous scan mode.

In Discrete mode Interval < 0 may provide faster data acquisition using inverse spacing. As an example let Min=400 nm, Max=800 and Interval=-10. The actual wavelength interval changes from 10 nm at 400 nm to 20 at 800. Negative Interval cannot be utilized in continuous scan mode.

Instead of a numerical range, you can enter the file name of a previously stored wavelength list created with **Setup...Wavelength List**. Click the label **List Name** to view the list of available files.

Measurement Type

Setup...Scan Method <Ctrl+M> (Screen 3A)

Specifies the type of data to be utilized in Baseline, Reference and Standard modes. Scanning is the only way to acquire data in Sample mode.

Constant

A constant cannot be used for Reference data in VW (VN for PE URA) mode.

File

Use data previously scanned and stored on disk.

Users must be certain that the utilization of previously stored data files does not adversely affect experimental accuracy.

Scan

Baseline or Reference data will be acquired by scanning. Data must be acquired before the Sample scan. The scan remains in memory until the program is exited.

Auto VN (mpe950.exe, PE URA only)

This Reference mode specifies that the PE Data Server will (as in *UV Win-Lab*) automatically normalize spectra. Only a Sample scan seems possible, but the 0% baseline (if Scan selected under Baseline) and 100% reference are measured but not displayed. That is, there are actually two or three scans for each sample scan. This mode is useful for a series of scans at different angles. The danger is that the user does not view reference scans, thereby eliminating visual verification that 'all is well'.

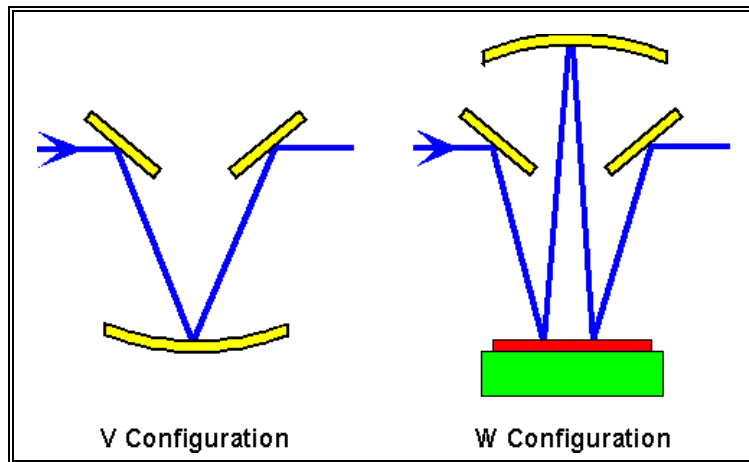
Program Mode

Setup...Scan Method <Ctrl+M> (Screen 2)

Select program mode and wavelength units. Wavelength units can only be selected in discrete scan mode.

Absorbance

Same as Transmittance mode except that the final graph is displayed with an optical density scale ($-\log_{10}(T)$).



VW Reflectance Attachment (not to scale)

V Reflectance

Single bounce reflectance attachment. An optic with known reflectance, typically an uncoated substrate, is placed on the reflectance attachment and scanned in Reference mode. The part is then removed and a coated part is inserted in the same position for the Sample scan. Accuracy is excellent for antireflection coatings.

VW Reflectance

Multiple bounce reflectance attachment. The Reference scan corresponds to the attachment set in 'V' configuration. The Sample scan corresponds to 'W' configuration. This technique is most accurate for high reflectors and is not recommended for AR coatings.

Wavelength List

Setup...Wavelength List...Edit

The Wavelength List editor creates and edits custom lists of scan wavelengths for Discrete Scan mode. This is useful when measuring laser mirrors and filters at discrete wavelengths. The maximum number of entries is the same as the maximum number of Sample data points specified in **Configuration...Capacity**.

Use **Edit...Generate** to add regularly spaced new wavelengths to the list. Use **Edit...Paste** to paste an Excel-generated column into the editor.

A list must be stored on disk before it can actually be used in a Scantraq scan. Be sure to set Scan Type to Discrete in Scan Method 1B and enter the file name under List in Scan Method 3B.

The list can also be used for interpolating digitized data (**Spectra...Convert Table**) when the SummaSketch digitizer is the input device.

Wavelength List Generator

from Wavelength List editor: Edit...Generate

The Wavelength Generator automatically inserts a table of wavelengths into the Wavelength List editor. Use it repeatedly to enter wavelengths over various ranges. This could be useful when scanning over blocking and bandpass zones where different intervals are appropriate for each region.

Interval<0 generates a list spaced inversely in wavelength. For example: 400-1200 X -10 nm. The spacing is 10 nm at 400 nm and increases to 30 nm at 1200 nm.

Spectra Menu

Data Table

Examine the measured spectrum. Disabled if there is no data to view. The table also calculates minimum, average and maximum values over a selected range. Click the column title to select the entire column.

Clear Data

Clear current spectral data from memory.

Smooth Data

Interactively set parameters for Moving Average (sometimes called boxcar or block average) or Savitzky-Golay (less smoothing but less spectral distortion) smoothing. Baseline and Reference scans use MA, while Sample scans utilize MA or S-G. MA is recommended for most purposes; S-G is recommended for sharp spectral peaks or edges.

***Smoothing averages data over adjacent wavelengths.
Smoothed data is not original data and may not be acceptable.
The interval must be small enough to retain spectral features.***

Auto Smooth

Check to automatically smooth Baseline, Reference and Sample scans using values set in the Smooth Data dialog. Before enabling, use the interactive Smooth Data dialog to verify that smoothing retains spectral features. This capability is especially useful for antireflection coatings.

Users who require different smoothing parameters for Baseline, Reference, and Sample scans can utilize BASIC Sub DataSmooth.

Copy/Paste Data

Transfer spectral data to and from other Windows applications via the clipboard.

DDE...Import/Export

Transfer spectral data to and from other Windows applications via DDE (dynamic data exchange).

Quick Save

Stores the current spectrum as "work.csv" which can then be opened in Excel and copied to an appropriate worksheet. Close "work.csv" before returning to Scantraq and repeating the procedure.

Auto Save OFF/ON

Turn on to automatically bring up the File Save As screen upon completing a scan. Excel models which control disk file storage can ensure that Auto Save is off with DDE command AUTOSAVE 0.

Convert Table

Using linear interpolation, convert an irregularly spaced tablet-digitized spectrum into a spectrum with regularly spaced wavelengths defined in Scan Method 3B - Measurement Range.

This is especially useful for averages or color measurements which are defined over particular wavelength intervals.

Graph Details...Line Color <Alt+R>

Spectral line color is most easily changed by clicking the Color Button at the lower right. Any spectrum in memory is replotted in the selected color. To *suppress* replotting hold down the shift key while clicking the button.

To change colors with the keyboard, press <Alt+R>, use left and right arrow keys to select and press <Enter>. Press <Shift+Alt+R> to change colors without replotting the current spectrum. Colors can also be selected with a single keystroke:

blac**K**, Red, Yellow, **B**lue, **G**reen, **M**agenta, **C**yan, **W**hite

There are two color palettes which are automatically selected according to the graph background. To suppress the dark palette click **Graph Details...No Dark Palette**.

Graph Details...Clip Plot

When this command is checked, spectral plots are 'clipped' and traces do not protrude beyond the graph axes. By turning off this function, replot speed may be increased on your computer. Speed is also increased by turning off the **Thick Line** selection.

Graph Details...Auto Color <Ctrl+U>, Auto Axes

Auto Color automatically selects a new line color when a spectrum is scanned, loaded, or pasted. This is useful for comparing spectra. **Auto Axes** automatically redraws new axes when a spectrum is scanned, loaded, or pasted. That is, only one spectrum can be viewed a time. Note that Auto Axes disables Auto Color.

Data Format

Clipboard

When examined with a text editor, sample transmittance data copied to the Windows clipboard appears as follows:

```
400  0    0.9876
450  0    0.9899
500  0    0.7891
```

Similarly, for Sample reflectance data:

```
400  0.0124  0
450  0.0111  0
500  0.2119  0
```

The first column is wavelength in nanometers followed by reflectance (0-1) and transmittance (0-1). Since we only measure reflectance or transmittance in Scantraq, the unmeasured quantity is set equal to zero. Data is TAB (ASCII 9) and CRLF delimited (ASCII 13 + ASCII 10) as follows:

```
400TAB0TAB0.9876CRLF
450TAB0TAB0.9899CRLF
```

Two-column data (wavelength and reflectance OR transmittance) can also be pasted. Data is pasted as reflectance or transmittance depending on graph axes setting. Uncheck **DESIGN Format** to copy in two-column format.

DDE

Data format is the same as tab-separated clipboard format discussed above. Data is transferred to a three column named cell block.

Format Options

As described above, spectra are normally copied and pasted (DDE transfer) with wavelength in nm. Check **Current units** to copy and paste spectra with the Wavelength Units currently specified in **Setup...Scan Method**. Normally reflectance and transmittance values are 0-1. Check **R & T in %** to change this to percent.

There are four file formats for loading and saving spectra. The first two file types are saved in ASCII format and can be read with a text editor. **.CSV** (comma-separated values) is Scantraq's default mode. **JCAMP** is a 'standard' which offers compatibility with spectroscopy software. **JCAMP + PerkinElmer compatible** should be used when saving PE Spectrum 2000 JCAMP files. The JCAMP standard is published in Robert S. McDonald and Paul A. Wilks Jr., *Applied Spectroscopy* **42**, 151 (1988).

Some programs deviate from published JCAMP standards or provide incomplete support. Programs frequently fail to support unequally-spaced wavelength data. Users who discover an incompatible JCAMP variation should contact FTG Software.

The third file format is binary .spc. This provides compatibility with Galactic Industries' *GRAMS* software. The fourth format is Excel .xls (Version 2.1). Excel files can be opened by Excel 97-2007.

Check **Combine reflectance and transmittance data** to keep both data arrays in memory for copying to the clipboard or storing on disk. Most importantly, both scans must have the same wavelength spacing. File format options are stored in the Scan Method.

.csv Format (File Open/Save)

When examined with a text editor, a Scantraq .csv file resembles the following (transmittance):

```
"Scantraq .csv format example"  
31  
450, .9975317  
460, .9985523  
470, .9986734  
etc.
```

The first line is an optional description (50 characters maximum); the line is included even if the description is blank. The second line is the number of spectral points. The third and subsequent lines are wavelength (nm), reflectance (0-1) and transmittance (0-1). If *For Excel* is checked the following is obtained:

```
450,0.9975313  
460,0.9985526  
470,0.9986742  
etc.
```

In Europe, users often set their computer's number settings (Control Panel Regional Settings) as follows: decimal symbol ",", digit grouping symbol (thousands separator) ".", list separator ";". In this case the Excel file looks like the following:

450;0,9975317
460;0,9985523
470;0,9986734
etc .

JCAMP and Scantraq .csv formats do not change when European number notation is used. Two-column data (wavelength and reflectance OR transmittance) can also be opened. Data is loaded as reflectance or transmittance depending on graph axes setting.

.xls (Excel) Format (File Open/Save)

Excel .xls format eliminates problems associated with .csv. While spectra can be opened in any version of Excel, Scantraq can only open Scantraq-created .xls spectra. Excel is not required.

W (nm)	%R
450	0.2528
460	0.146188
470	0.13243
480	0.15352

Users with more complex requirements, for example exporting multiple spectra to a single Excel file, can utilize a Scantraq BASIC macro. In that case, however, Excel must be installed.

Standard Data Editor

Spectra...Data Editor

This editor enables users to input Standard data from published tables. The editor is only available when Standard data is specified in **Spectra...Data Type**. The dialog box becomes a data viewer when other data types are specified. (To help maintain data integrity Scantraq does not permit users to edit scanned data.) Standard data can also be pasted from the clipboard (**<Ctrl+V>**) or loaded from Excel-compatible files.

Using the grid control, users can enter the same values in all or part of the reflectance or transmittance column by highlighting the range before typing values. Select the entire column by clicking the column title. For example to enter 4.2% in all rows, click the title '% Refl' and type '4.2'. Entries can be deleted by selecting entire rows and pressing ****.

Tablet Procedures

The Mpe983.exe version of Scantraq supports data entry with Summagraphics SummaSketch digitizer tablets.

Strip-Chart Alignment - 1

Tape the strip-chart spectrum to the tablet surface and enter wavelengths corresponding to left and right boundaries. The strip-chart need not be mounted perfectly parallel to the tablet edge. If the chart is bigger than the tablet, it will be possible to acquire data as a series of separate scans.

Strip-Chart Alignment - 2

Locate and enter points in the following order:

1. Lower Left
2. Lower Right

