

# Exporting Data from the Agilent 8453E UV-visible Spectroscopy System to a Personal Computer

# **Technical Note**

# Introduction

The Agilent 8453E UV-visible spectroscopy system is a standalone system, comprising an Agilent 8453 spetrophotometer and handheld controller. The controller is used to process measurement data and results can be reviewed, saved or printed when a printer is connected to the system.

For further processing of measurement data such as adding and comparing results to those acquired on other systems, or for preparing reports with customized layouts, the Agilent 8453E system provides for transfer of data to a personal computer using a PC card.

This technical note describes in detail how to export data from the Agilent 8453E system to a variety of PC applications.

## Equipment

The data transfer described in this note was carried out using the following equipment.

- Agilent 8453E UV-visible spectroscopy system, comprising spectrophotometer and handheld controller.
- HP Kayak PC with PC-card adapter.
- Agilent ChemStation software for UV-visible spectroscopy (revision

## Before you begin

Make sure the PC card is inserted in the handheld controller before you turn on line power at the spectrophotometer. If you insert a PC card after turning on line power, you will not be able to save data on the PC card.





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# Data types and file structures

# **Spectrum files**

Except for kinetic measurements the Agilent 8453E saves results of all tasks in ASCIIformat files with the extension .wav. Spectra of either samples or standards can be saved. Figure 1 shows the basic structure of a spectrum file. For more information on the file structure, see the *Agilent 8453E User Manual.* 



#### Figure 1

Figure 2

Basic structure of a spectrum file (.wav)



#### **Kinetics files** The Agilent 8453E saves

results of kinetic measurements (timetraces) in ASCIIformat files with the extension .csv. Figure 2 shows the basic structure of a kinetics file. For more information on the file structure, see the *Agilent 8453E User Manual*.

## Saving data to the PC card

- 1. Use the up and down arrow keys to select sample, standard or timetrace from the results table.
- 2. Press the **m** key.
- 3. Select item **Export select**ed sample, see figure 3.
- 4. Type a name of up to eight characters (without the extension) for the file as shown in figure 4.
- 5. Press **Save As** and then press **Done** to exit the window.



Figure 3

Selecting the data you want to export

Basic structure of a kinetics file (.csv)



Figure 4 Saving the data in a file

The selected spectrum is now saved on your PC card.

- 1. Remove the PC card from the controller and insert it into the PC-card-drive of your PC.
- 2. Use Microsoft<sup>®</sup> Explorer to copy the file to a folder of your choice on your PC.

# Importing spectra into Agilent ChemStation

To open your files, choose **Import** from the **File** menu and then choose **Samples**, **Standards** or **Auxiliary**, see figure 5.

You can handle and process imported data in the same way as data acquired with the Agilent ChemStation. Note that you can import spectrum files only—this feature is not appli-cable for kinetics files.

# Opening your files with editors, spreadsheets or data analysis applications

You can open spectrum or kinetics files as unformatted text using editors such as Microsoft Notepad or Wordpad. You can apply the following procedure for most applications:

- 1. Use the **Open** command from the **File** menu.
- 2. Process the imported data using the features of your chosen application.



Figure 5 Inporting the data into Agilent ChemStation

Some data analysis applications sort the data automatically into rows and columns. With these applications you may encounter problems addressing the correct cells. As a consequence data may be lost or sorted in a wrong way.

Use the following procedure as a workaround for these problems:

1. Open the files using an application that handles the data correctly, as described above.

- 2. Copy all the data to the Clipboard, using the **Select All** command from the **Edit** menu and then the **Copy** command from the **Edit** menu.
- 3. Use the **Paste** command from the **Edit** menu to put the data from the clipboard into the application that was unable to open the files correctly.

# Importing into Microsoft Excel

- 1. Use **Open** from the **File** menu to import data from spectrum files as Excel tables. Excel recognizes that the data is delimited, see figure 6.
- 2. Set **Comma** as delimiter, that is, the character that separates different columns, see figure 7.
- 3. Insert a column before the first column to create place for the wavelengths of the data points (select a cell in the first column and then use **Columns** from the **Insert** menu.)
- 4. Add the wavelengths by typing the values in the new column. The wavelength range is given in line 8 of the file header, see also figure 1. Use **Fill-Series** in the **Edit** menu to fill the additional measurement points (select **Series in Columns** and enter a **Step value** and **Stop value**, see figure 8.)

You now have a complete data set for further processing, comprising wavelengths (in column 1) and measured data values (in column 2.)

Note that kinetics files are automatically recognized by Excel and opened with the appropriate delimiters.



#### Figure 6

Excel recognizes that the data is delimited

Text Import ₩izard - Step 2 of 3	? ×			
This screen lets you set the delimiters your data contains. You can see how your text is affected in the preview below.				
Delimiters	Treat consecutive delimiters as one			
	Text Qualifier:			

#### Figure 7

#### Set Comma as the delimiter

Series			? ×
Series in O Rows O <u>C</u> olumns	Type © Linear © Growth © Date	Date unit © Day C Weekday C Month	OK Cancel
Trend	C Auto <u>Fill</u> St <u>o</u> p val	C Year	

Figure 8

Adding the wavelength values

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