



# USB4000 Fiber Optic Spectrometer

## Installation and Operation Manual

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# About This Manual

## Document Purpose and Intended Audience

This document provides the users of USB4000 Spectrometers with instructions for setting up, calibrating and performing experiments with their spectrometer.

## What's New in This Document

This version of the *USB4000 Fiber Optic Spectrometer Installation and Operation Manual* removes the N and P designations from some of the pins in the Accessory Connector Pinout Table.

## Document Summary

Chapter	Description
Chapter 1: <a href="#">Introduction</a>	Contains descriptive information about the USB4000 Spectrometer and how sampling works. It also provides a list of system requirements, interface options, and shipment components.
Chapter 2: <a href="#">Installing the USB4000</a>	Provides installation instructions.
Chapter 3: <a href="#">Troubleshooting</a>	Contains recommended steps to isolate and correct common problems.
Chapter 4: <a href="#">Sample Experiments</a>	Offers instructions for preparing for and taking measurements with the USB4000 Spectrometer.
Appendix A: <a href="#">Calibrating the Wavelength of the USB4000</a>	Provides instructions for calibrating the USB4000 Spectrometer.
Appendix B: <a href="#">External Triggering</a>	Contains information about external triggering for the USB4000.
Appendix C: <a href="#">Specifications</a>	Contains technical specifications and connector pinouts for the USB4000 Spectrometer.

## Product-Related Documentation

You can access documentation for Ocean Optics products by visiting our website at <http://www.oceanoptics.com>. Select *Technical* → *Operating Instructions*, then choose the appropriate document from the available drop-down lists. Or, use the **Search by Model Number** field at the bottom of the web page.

- Detailed instructions for the SpectraSuite Spectrometer Operating Software are located at: <http://www.oceanoptics.com/technical/SpectraSuite.pdf>.

Engineering-level documentation is located on our website at *Technical* → *Engineering Docs*.

You can also access operating instructions for Ocean Optics products from the *Software and Technical Resources* CD that ships with the product.

## Upgrades

Occasionally, you may find that you need Ocean Optics to make a change or an upgrade to your system. To facilitate these changes, you must first contact Customer Support and obtain a Return Merchandise Authorization (RMA) number. Please contact Ocean Optics for specific instructions when returning a product.

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## Chapter 1

# Introduction

## Product Overview

The Ocean Optics USB4000 Spectrometer is our next generation, high-performance, miniature fiber-optic spectrometer designed from our popular USB2000 model to include an advanced detector and powerful high-speed electronics. New features consist of the 3648-element detector with shutter, high-speed electronics, and interface capabilities to Linux, Macintosh and Windows operating systems. The USB4000 is responsive from 200-1100 nm, but the specific range and resolution depends on your grating and entrance slit selections.

The USB4000 is perfect for applications where enhanced electronics, high resolution and fast integration times are required.

Data programmed into a memory chip on each USB4000 includes wavelength calibration coefficients, linearity coefficients, and the serial number unique to each spectrometer. Our spectrometer operating software simply reads these values from the spectrometer — a feature that enables hot swapping of spectrometers among computers.

The USB4000 Spectrometer connects to a computer via the USB port or serial port. When connected through a USB 2.0 or 1.1, the spectrometer draws power from the host computer, eliminating the need for an external power supply. The USB4000, like all USB devices, can be controlled by our SpectraSuite software, a completely modular, Java-based spectroscopy software platform that operates on Windows, Macintosh and Linux operating systems.



**Ocean Optics USB4000 Fiber Optic Spectrometer**

# Features

- ❑ TCD1304AP Detector
- ❑ Responsive from 200 to 1100 nm, specific range and resolution depends on your grating and entrance slit choices
- ❑ Sensitivity of up to 130 photons/count at 400 nm; 60 photons/count at 600 nm
- ❑ An optical resolution of ~0.3 (FWHM)
- ❑ A wide variety of optics available
  - 14 gratings
  - 6 slit widths
  - 3 detector coatings
  - 6 optical filters
- ❑ Integration times from 10  $\mu$ s to 65 seconds
- ❑ Embedded microcontroller allows programmatic control of all operating parameters and standalone operation
  - USB 2.0 480Mbps (high speed) and 12Mbps (full speed)
  - RS232 115K baud
  - Multiple communication standards for digital accessories (SPI, I<sup>2</sup>C)
- ❑ EEPROM storage for
  - Wavelength Calibration Coefficients
  - Linearity Correction Coefficients
  - Absolute Irradiance Calibration (optional)
- ❑ Low power consumption of only 250 mA @ 5 VDC
- ❑ 16 bit, 3MHz A/D Converter
- ❑ 5 triggering modes
- ❑ 2 programmable strobe signals for triggering other devices
- ❑ 24-pin connector for interfacing to external products
- ❑ Programmable for Standalone Operation
- ❑ CE Certification

# System Requirements

You can use the USB4000's USB connectivity with any computer that meets the following requirements:

- Operating system is one of the following:
  - Windows – 98/Me/2000/XP
  - Apple Macintosh – OS X version 10.0 or later
  - Linux – Red Hat 9 or later, Fedora (any version), Debian 3.1 (Sarge), and SUSE (9.0 or later)
- Ocean Optics' SpectraSuite software application installed and configured for use with the USB4000.

## EEPROM Utilization

An EEPROM memory chip in each USB4000 contains wavelength calibration coefficients, linearity coefficients, and a serial number unique to each individual spectrometer. The SpectraSuite software application reads these values directly from the spectrometer, enabling the ability to “hot-swap” spectrometers between computers without entering the spectrometer coefficients manually on each computer.

## About SpectraSuite

SpectraSuite is a completely modular, Java-based spectroscopy software platform that operates on Windows, Macintosh and Linux operating systems. The software can control any Ocean Optics USB spectrometer and device, as well as any other manufacturer's USB instrumentation using the appropriate drivers. SpectraSuite is a user-customizable, advanced acquisition and display program that provides a real-time interface to a variety of signal-processing functions. With SpectraSuite, you have the ability to perform spectroscopic measurements (such as absorbance, reflectance, and emission), control all system parameters, collect and display data in real time, and perform reference monitoring and time acquisition experiments.

## Sampling System Overview

### How Sampling Works

Ocean Optics components function in a sampling system as follows:

1. The user stores reference and dark measurements to correct for instrument response variables.
2. The light from the light source transmits through an optical fiber to the sample.
3. The light interacts with the sample.
4. Another optical fiber collects and transmits the result of the interaction to the spectrometer.
5. The spectrometer measures the amount of light and transforms the data collected by the spectrometer into digital information.

6. The spectrometer passes the sample information to SpectraSuite.
7. SpectraSuite compares the sample to the reference measurement and displays processed spectral information.

## Modular Light Sources and Sampling Accessories

Ocean Optics offers a complete line of spectroscopic accessories for use with the USB4000. Most of our spectroscopic accessories have SMA connectors for application flexibility. Accordingly, changing the sampling system components is as easy as unscrewing a connector and replacing an accessory. Available accessories include the following:

- USB-ISS-UV-VIS Integrated Sampling System for Cuvettes (200–1100 nm)
- USB-ISS-VIS Integrated Sampling System for Cuvettes (390–900 nm)
- USB-LS-450 Pulsed Blue LED Module
- USB-DT Deuterium Tungsten Light Source (200–2000 nm)
- HR4-BREAKOUT Breakout Box for Controlling Devices (see [Breakout Box](#))

## Interface Options

The USB4000 has both USB and serial port connectors (with the use of an adapter), enabling you to connect the spectrometer to a computer via a USB or serial port. However, you must create custom software if using the serial port. SpectraSuite software is available if you are connecting via the USB port.

## Breakout Box

Ocean Optics also offers the Breakout Box (HR4-BREAKOUT), a passive module that separates the signals from their 22-pin port to an array of standard connectors and headers, enabling easy access to a variety of features found in Ocean Optics' USB4000 Spectrometer. In addition to the accessory connector, the breakout box features a circuit board based on a neutral breadboard pattern that allows custom circuitry to be prototyped on the board itself.

## Shipment Components

The following information and documentation ships with the USB4000 Spectrometer:

### ❑ Packing List

The packing list is inside a plastic bag attached to the outside of the shipment box (the invoice arrives separately). It lists all items in the order, including customized components in the spectrometer (such as the grating, detector collection lens, and slit). The packing list also includes the shipping and billing addresses, as well as any items on back order.

### ❑ USB Cable (USB-CBL-1)

Use this cable to connect your spectrometer to a computer running on a Windows, Mac or Linux operating system.

❑ **Wavelength Calibration Data Sheet**

Each spectrometer is shipped with a Wavelength Calibration Data Sheet that contains information unique to your spectrometer. SpectraSuite Operating Software reads this calibration data from your spectrometer when it interfaces to a computer via the USB port.

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**Note**

Please save the Wavelength Calibration Data Sheet for future reference.

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❑ **Software and Technical Resources CD**

Each order ships with the Ocean Optics *Software and Resources CD*. This disc contains software, operating instructions, and product information for all Ocean Optics software, spectrometers, and spectroscopic accessories. You need Adobe Acrobat Reader version 6.0 or higher to view these files. Ocean Optics includes the Adobe Acrobat Reader on the *Software and Technical Resources CD*.

Ocean Optics software requires a password during the installation process. You can locate passwords for the other software applications on the back of the *Software and Technical Resources CD* package.

## Additional Equipment Needed

❑ **SpectraSuite Operating Software**

See [About SpectraSuite](#) for more information.

## Other Accessories Available

Visit us at [www.OceanOptics.com](http://www.OceanOptics.com) for a complete list of products available for all of your spectroscopy needs.

- ❑ **Fibers**
- ❑ **Light Sources**
- ❑ **Integrated Sampling Systems**
- ❑ **Cuvettes**
- ❑ **Filter Holders**
- ❑ **Lithium Ion Battery Pack**
- ❑ **HR4-BREAKOUT Breakout Box**

See [Breakout Box](#) for more information.



# Installing the USB4000

## Overview

You must install the SpectraSuite software application prior to connecting the USB4000 Spectrometer to the computer. The SpectraSuite software installation installs the drivers required for USB4000 installation. If you do not install SpectraSuite first, the system will not properly recognize the USB4000.

If you have already connected the USB4000 to a computer running on a Windows platform prior to installing SpectraSuite, consult *Chapter 3: [Troubleshooting](#)* for information on correcting a corrupt USB4000 installation.

## USB4000 Installation

This section contains instructions for connecting the USB4000 via both USB and serial modes.

### USB Mode

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#### Note

The USB port on a computer can power up to five USB4000 spectrometer channels. Systems with more than five channels require a powered USB hub.

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#### ► Procedure

Follow the steps below to connect the USB4000 to a computer via the USB port:

1. Install SpectraSuite on the destination computer.
2. Locate the USB cable (USB-CBL-1) provided with the USB4000.
3. Insert the square end of the cable into the side of the USB4000.
4. Insert the rectangular end of the cable into the USB port of the computer.

If you installed SpectraSuite prior to connecting the USB4000, the **Add New Hardware Wizard** appears and installs the USB4000 drivers. If the drivers do not successfully install (or if you connected the USB4000 to the computer before installing SpectraSuite), consult *Chapter 3: [Troubleshooting](#)*.

## Serial Port Mode

To use the serial port capacity of the USB4000 Spectrometer, the computer must be running a 32-bit version of the Windows operating system.

### ► **Procedure**

Follow the steps below to connect the USB4000 to the computer via serial port:

1. Connect the serial cable adapter block to the appropriate pins of the USB4000's 30-Pin Accessory Connector.
2. Connect one end of the 9-pin serial cable to the adapter block on the USB4000, and then connect the other end to a serial port on the computer.
3. Note the number of the serial port (COM Port) to which you connected the USB4000 (some computers may not have numbered ports; handheld computers typically have only one serial port).
4. Plug the 5 VDC external power supply into an outlet and connect it to the USB4000.

## Connect Spectroscopic Accessories

To find operating instructions for USB4000-compatible products (such as light sources, sampling chambers, and probes), consult the *Software and Technical Resources* CD or the Ocean Optics website at <http://www.oceanoptics.com/technical/operatinginstructions.asp>.

## External Triggering Options

You can trigger the USB4000 using a variety of External Triggering options through the 22-pin Accessory Connector on the spectrometer. See Appendix B: [External Triggering](#) for more information.

# Troubleshooting

## Overview

The following sections contain information on troubleshooting issues you may encounter when using the USB4000 Spectrometer.

## USB4000 Connected to Computer Prior to SpectraSuite Installation

### Windows Operating Systems

If you connected your Ocean Optics USB4000 device to the computer prior to installing your Ocean Optics software application on a Windows platform, you may encounter installation issues that you must correct before your Ocean Optics device will operate properly.

Follow the applicable steps below to remove the incorrectly installed device, device driver, and installation files.

---

#### Note

If these procedures do not correct your device driver problem, you must obtain the *Correcting Device Driver Issues* document from the Ocean Optics website:  
<http://www.oceanoptics.com/technical/engineering/correctingdevicedriverissues.pdf>.

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### Remove the Unknown Device from Windows Device Manager

#### ► Procedure

1. Open Windows Device Manager. Consult the Windows operating instructions for your computer for directions, if needed.
2. Locate the **Other Devices** option and expand the **Other Devices** selection by clicking on the "+" sign to the immediate left.

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### Note

Improperly installed USB devices can also appear under the Universal Serial Bus Controller option. Be sure to check this location if you cannot locate the unknown device.

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3. Locate the unknown device (marked with a large question mark). Right-click on the **Unknown Device** listing and select the **Uninstall** or **Remove** option.
4. Click the **OK** button to continue. A warning box appears confirming the removal of the Unknown Device. Click the **OK** button to confirm the device removal.
5. Disconnect the USB4000 from your computer.
6. Locate the section in this chapter that is appropriate to your operating system and perform the steps in the following [Remove Improperly Installed Files](#) section.

## Remove Improperly Installed Files

### ► Procedure

1. Open Windows Explorer.
2. Navigate to the **Windows | INF** directory.

---

### Note

If the INF directory is not visible, you must disable the Hide System Files and Folders and Hide File Extensions for Known File Types options in Windows Folder Options. Access Windows Folder Options from Windows Explorer, under the **Tools | Folder Options** menu selection.

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3. Delete the **OOI\_USB.INF** in the INF directory. If your computer is running either the Windows 2000 or XP operating system, you must also delete the **OOI\_USB.PNF** file in the INF directory.
4. Navigate to the **Windows | System32 | Drivers** directory.
5. Delete the **EZUSB.SYS** file.
6. Reinstall your Ocean Optics application and reboot the system when prompted.
7. Plug in the USB device.

The system is now able to locate and install the correct drivers for the USB device.

## Mac Operating Systems

Since there are no device files for the USB4000 Spectrometer in a Mac operating system, you should not encounter any problems if you installed the spectrometer before the SpectraSuite software.

## Linux Operating Systems

For Linux operating systems, all you need to do is install the SpectraSuite software, then unplug and replug in the spectrometer. Technically, the driver files for Linux simply give nonprivileged users permission to use newly connected hardware. There isn't any long-term harm to plugging in the device before installing the software.



# Sample Experiments

## Overview

The following sections list instructions for conducting several sample experiments using the USB4000 Spectrometer with SpectraSuite software. The *SpectraSuite Spectrometer Operating Software Installation and Operation Manual* contains more information on experiments (see [Product-Related](#) Documentation).

## Preparing for Experiments

Follow the procedure below to configure the USB4000 and SpectraSuite for experiments.

### ► Procedure

1. Double-check that you have correctly installed the USB4000, installed SpectraSuite, and configured the light source and other sampling optics.
2. Open the SpectraSuite application.
3. Adjust the acquisition parameters using the **Acquisition Parameters** dialog bar or select **Spectrum | Configure Data Acquisition** from the menu.

If you have followed the previous steps and started SpectraSuite, the spectrometer is already acquiring data. Even with no light in the spectrometer, there should be a dynamic trace displayed in the bottom of the graph. If you allow light into the spectrometer, the graph trace should rise with increasing light intensity. This means the software and hardware are correctly installed.

Note the spectrometer(s) that you have installed are listed in the Data Sources pane.

Once you install the software and hardware, and establish your sampling system, you are ready to take measurements.

## Taking Measurements

This section describes how to conduct the following basic optical measurements:

- Absorbance (see [Absorbance Experiments](#))
- Transmission (see [Transmission Experiments](#))
- Reflection (see [Reflection Experiments](#))
- Relative irradiance (see [Relative Irradiance Experiments](#))

## 4: Sample Experiments

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The type of measurement you take determines the configuration of the sampling optics for your system. Furthermore, your choice of reference and data analysis determines how the SpectraSuite presents the results.

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### Note

For each measurement, you must first take a reference scan and a dark spectrum scan. After you take a reference scan and a dark spectrum scan, you can take as many measurement scans as needed. However, if you change any sampling variable (integration time, averaging, smoothing, angle, temperature, fiber size, etc.), you must store new reference and dark spectrum scans.

---

## Application Tips

If the signal you collect is saturating the spectrometer (intensity greater than 65535 counts), you can decrease the light level on scale in scope mode by:

- Decreasing the integration time
- Attenuating the light going into the spectrometer
- Using a smaller diameter fiber
- Using a neutral density filter with the correct optical density

If the signal you collect has too little light, you can increase the light level on scale in scope mode by:

- Increasing the integration time
- Using a larger diameter fiber
- Removing any optical filters

## Absorbance Experiments

Absorbance spectra are a measure of how much light a sample absorbs. For most samples, absorbance is linearly related to the concentration of the substance. SpectraSuite calculates absorbance ( $A_\lambda$ ) using the following equation:

$$A_\lambda = - \log_{10} \left( \frac{S_\lambda - D_\lambda}{R_\lambda - D_\lambda} \right)$$

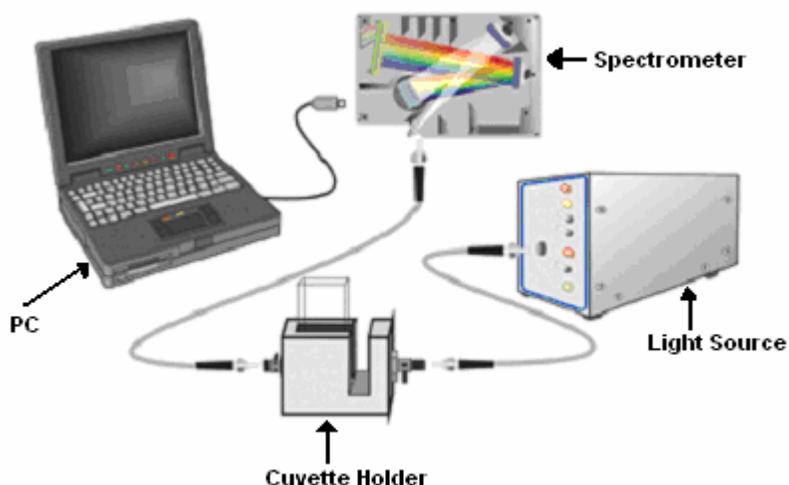
Where:

$S_\lambda$  = the sample intensity at wavelength  $\lambda$

$D_\lambda$  = the dark intensity at wavelength  $\lambda$

$R_\lambda$  = the reference intensity at wavelength  $\lambda$

The figure below shows a typical absorbance setup. The light source sends light via an input fiber into a cuvette in a cuvette holder. The light interacts with the sample. The output fiber carries light from the sample to the spectrometer, which is connected to the computer.



### Typical Absorbance Setup

Absorbance is also proportional to the concentration of the substance interacting with the light (this is known as Beer's Law). Common absorption applications include the quantification of chemical concentrations in aqueous or gaseous samples.

#### ► Procedure

To take an absorbance measurement using SpectraSuite, follow the steps below:

1. Place SpectraSuite in Scope mode by clicking the Scope (  ) icon in the Experiment mode toolbar or selecting **Processing | Processing Mode | Scope** from the menu.
2. Ensure that the entire signal is on scale. The intensity of the reference signal should peak at about 50000 counts. If necessary, adjust the integration time until the intensity is approximately 50000 counts.
3. If you have not already done so, place a sample of the solvent into a cuvette and take a reference spectrum. You must take a reference spectrum before measuring absorbance.

---

#### Note

Do not put the sample itself in the path when taking a reference spectrum, only the solvent.

---

Click the Store Reference Spectrum (  ) icon on the toolbar or by select **File | Store | Store Reference Spectrum** from the menu bar to store the reference. This command merely stores a reference spectrum in memory. You must click the Save Spectra (  ) icon on the toolbar or select **File | Save | Save Spectra Collection** from the menu bar to permanently save the reference spectrum to disk.

#### 4: Sample Experiments

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- If you have not already done so, store a dark spectrum reading. To do this, block the light path to the spectrometer, uncheck the **Strobe/Lamp Enable** box in the Acquisition toolbar, or turn the light source off. Then, take a dark spectrum by clicking the Store Dark Spectrum () icon on the toolbar or by selecting **File | Store | Store Dark Spectrum** from the menu bar. This command merely stores a dark spectrum in memory. You must click the Save Spectra () icon on the toolbar or select **File | Save | Save Spectra Collection** from the menu bar to permanently save the spectrum to disk.

---

#### Note

If possible, do not turn off the light source when taking a dark spectrum. If you must turn off your light source to store a dark spectrum, allow enough time for the lamp to warm up again before continuing your experiment. After the lamp warms up again, store a new reference (Step 3).

---

You must take a dark spectrum before measuring absorbance.

- Put the sample in place and ensure that the light path is clear. Then, take an absorbance measurement by clicking on the Absorbance () icon on the toolbar or selecting **Processing | Processing Mode | Absorbance** from the menu. Note the following changes on the screen:
  - The experiment mode listed in the Data Sources and Data Views panes changes to Absorbance Mode.
  - The units listed on the Graph pane changes to Absorbance (OD).
- To permanently save the spectrum to disk, click the Save Spectra () icon on the toolbar.

---

#### Note

If you change any sampling variable (integration time, averaging, smoothing, fiber size, etc.), you must store a new dark and reference spectrum.

---

## Transmission Experiments

Transmission is the percentage of energy passing through a sample relative to the amount that passes through the reference. Transmission Mode also displays the portion of light *reflected* from a sample, since transmission and reflection measurements use the same mathematical calculations. The transmission is expressed as a percentage (%T<sub>λ</sub>) relative to a standard substance (such as air). SpectraSuite calculates %T<sub>λ</sub> (or %R<sub>λ</sub>) with the following equation:

$$\%T_{\lambda} = \frac{S_{\lambda} - D_{\lambda}}{R_{\lambda} - D_{\lambda}} \times 100\%$$

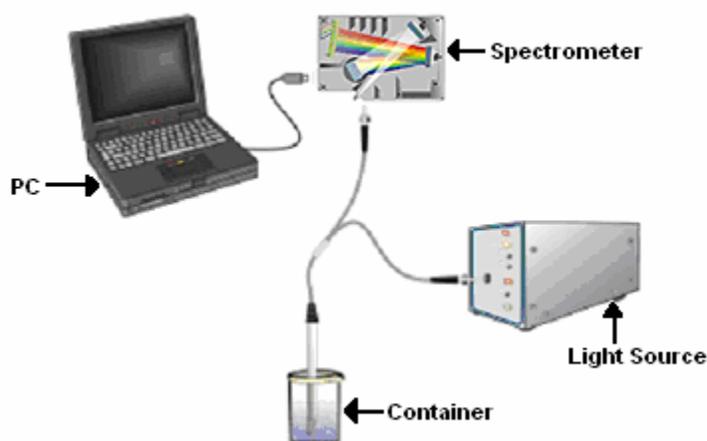
Where:

$S_\lambda$  = the sample intensity at wavelength  $\lambda$

$D_\lambda$  = the dark intensity at wavelength  $\lambda$

$R_\lambda$  = the reference intensity at wavelength  $\lambda$

The following figure shows a typical transmission setup. The light source sends light via the input leg of a transmission probe into a container. The light interacts with the sample. The output leg of the transmission probe carries the information to the spectrometer, which transmits the information to the computer.



**Typical Transmission Setup**

Common transmission applications include measuring light through solutions, optical filters, optical coatings, and other optical elements (such as lenses and fibers).

► **Procedure**

Perform the following steps to take a transmission measurement using SpectraSuite:

1. Place SpectraSuite in Scope mode by clicking the Scope (  ) icon in the Experiment mode toolbar or selecting **Processing | Processing Mode | Scope** from the menu.
2. Ensure that the entire signal is on scale. The intensity of the reference signal should peak at about 50000 counts. If necessary, adjust the integration time until the intensity is approximately 50000 counts.
3. If you have not already done so, place a sample of the solvent into a cuvette and take a reference spectrum. You must take a reference spectrum before measuring transmission.

---

### Note

Do not put the sample itself in the path when taking a reference spectrum, only the solvent.

---

Click the Store Reference Spectrum () icon on the toolbar or by select **File | Store | Store Reference Spectrum** from the menu bar to store the reference. This command merely stores a reference spectrum in memory. You must click the Save Spectra () icon on the toolbar to permanently save the reference spectrum to disk.

4. If you have not already done so, store a dark spectrum reading. To do this, block the light path to the spectrometer, uncheck the **Strobe/Lamp Enable** box in the Acquisition toolbar, or turn the light source off. Then, take a dark spectrum by clicking the Store Dark Spectrum () icon on the toolbar or by selecting **File | Store | Store Dark Spectrum** from the menu bar. This command merely stores a dark spectrum in memory. You must click the Save Spectra () icon on the toolbar or select **File | Save | Save Spectra Collection** from the menu bar to permanently save the spectrum to disk.
- 

### Note

If possible, do not turn off the light source when taking a dark spectrum. If you must turn off your light source to store a dark spectrum, allow enough time for the lamp to warm up again before continuing your experiment.

---

You must take a dark spectrum before measuring transmission.

5. Put the sample in place and ensure that the light path is clear. Then, take a transmission measurement by clicking on the Transmission () icon on the toolbar or selecting **Processing | Processing Mode | Transmission** from the menu. Note the following changes on the screen:
    - The experiment mode listed in the Data Sources and Data Views panes changes to **Transmission Mode**.
    - The units listed on the Graph pane changes to **Transmission (%)**.
  6. To permanently save the spectrum to disk, click the Save Spectra () icon on the toolbar or select **File | Save | Save Spectra Collection** from the menu bar.
- 

### Note

If you change any sampling variable (integration time, averaging, smoothing, fiber size, etc.), you must store a new dark and reference spectrum.

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# Reflection Experiments

Reflection is the return of radiation by a surface, without a change in wavelength. Reflection can be:

- Specular (the angle of incidence is equal to the angle of reflection)
- Diffuse (the angle of incidence is not equal to the angle of reflection)

Every surface returns both specular and diffuse reflections. Some surfaces may return mostly specular reflection, while others may return mostly diffuse reflection. Specular reflection increases proportionately with the amount of gloss on a surface.

Reflection is expressed as a percentage (% $R_\lambda$ ) relative to the reflection from a standard reference substance:

$$\%R_\lambda = \frac{S_\lambda - D_\lambda}{R_\lambda - D_\lambda} \times 100\%$$

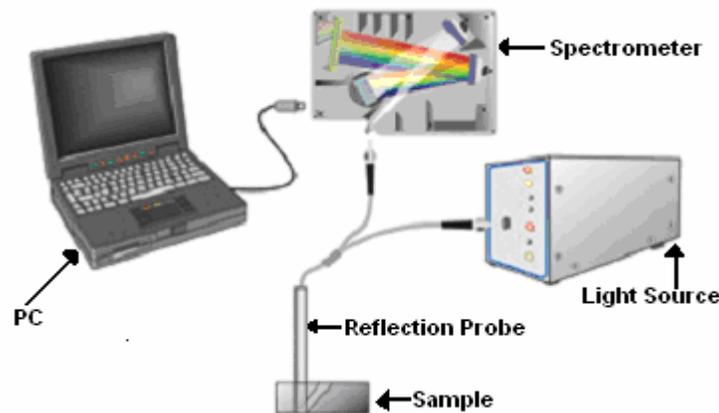
Where:

$S_\lambda$  = the sample intensity at wavelength  $\lambda$

$D_\lambda$  = the dark intensity at wavelength  $\lambda$

$R_\lambda$  = the reference intensity at wavelength  $\lambda$

The following figure shows a typical reflection setup. A light source sends light via the input leg of a reflection probe onto a sample. A reflection probe holder holds the probe in either a 90 or 45-degree angle from the surface. The output leg of the reflection probe carries light from the sample to the spectrometer, which is connected to the computer.



Typical Reflection Setup

Common reflection applications include measuring the properties of mirrors and coatings. Other applications include measuring the visual properties of the color in paints, plastics, and food products.

### ► Procedure

Perform the following steps to take reflection measurements using SpectraSuite:

1. Place SpectraSuite in Scope mode by clicking the Scope () icon in the Experiment mode toolbar or selecting **Processing | Processing Mode | Scope** from the menu.
2. Ensure that the entire signal is on scale.
3. Take a reference spectrum with the WS-1 Diffuse Reflectance Standard or the STAN-SSH High-reflectivity Reference Standard. You must take a reference spectrum before measuring reflection.

Click the Store Reference Spectrum () icon on the toolbar or by select **File | Store | Store Reference Spectrum** from the menu bar to store the reference. This command merely stores a reference spectrum in memory. You must click the Save Spectra () icon on the toolbar to permanently save the reference spectrum to disk.

4. Either block the light path to the spectrometer, uncheck the **Strobe/Lamp Enable** box in the Acquisition toolbar, or turn the light source off. Then, take a dark spectrum by clicking the Store Dark Spectrum () icon on the toolbar or by selecting **File | Store | Store Dark Spectrum** from the menu bar. This command merely stores a dark spectrum in memory. You must click the Save Spectra () icon on the toolbar or select **File | Save | Save Spectra Collection** from the menu bar to permanently save the spectrum to disk.

---

#### Note

If possible, do not turn off the light source when taking a dark spectrum. If you must turn off your light source to store a dark spectrum, allow enough time for the lamp to warm up again before continuing your experiment.

---

You must take a dark spectrum before measuring reflection.

5. Put the sample in place and ensure that the light path is clear. Then, take a reflection measurement by clicking on the Transmission () icon on the toolbar or selecting **Processing | Processing Mode | Transmission** from the menu (since the mathematical calculations used to calculate transmission and reflection are identical). To permanently save the spectrum to disk, click the Save Spectra () icon on the toolbar or select **File | Save | Save Spectra Collection** from the menu bar.

---

#### Note

If you change any sampling variable (integration time, averaging, smoothing, angle, temperature, fiber size, etc.), you must store a new dark and reference spectrum.

---

# Relative Irradiance Experiments

Irradiance is the amount of energy at each wavelength emitted from a radiant sample. In relative terms, it is a comparison of the fraction of energy the sample emits and the energy the sampling system collects from a lamp with a blackbody energy distribution (normalized to 1 at the energy maximum). SpectraSuite calculates relative irradiance with the following equation:

$$I_{\lambda} = B_{\lambda} \left( \frac{S_{\lambda} - D_{\lambda}}{R_{\lambda} - D_{\lambda}} \right)$$

Where:

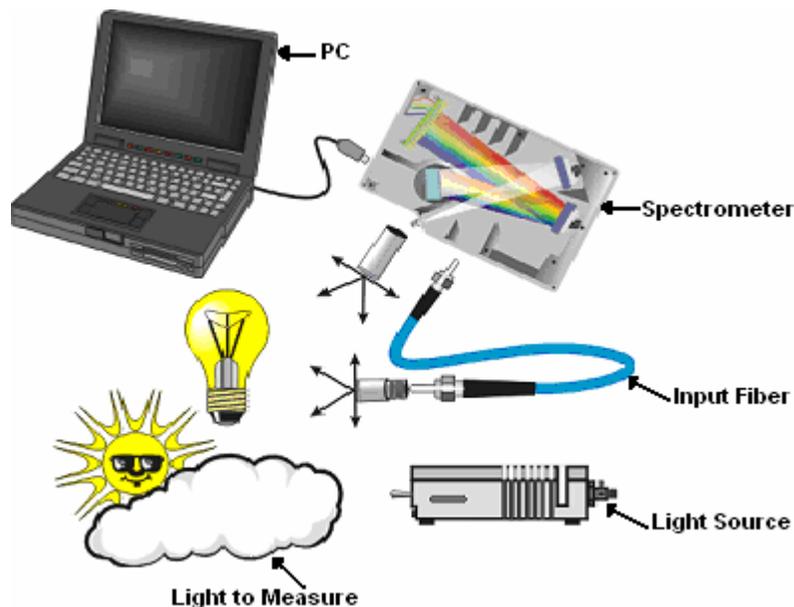
$B_{\lambda}$  = the relative energy of the reference (calculated from the color temperature) at wavelength  $\lambda$

$S_{\lambda}$  = the sample intensity at wavelength  $\lambda$

$D_{\lambda}$  = the dark intensity at wavelength  $\lambda$

$R_{\lambda}$  = the reference intensity at wavelength  $\lambda$

The following figure shows a typical relative irradiance setup. A light source with a known color temperature (such as the LS-1 or LS-1-LL) is used to take a reference spectrum. The light to measure is accumulated through a CC-3 Cosine Corrector (or FOIS integrating sphere) into an input fiber, which carries the light information to the spectrometer. The spectrometer then transmits the information to the computer, which compares the measured spectra against the reference spectrum, thus removing wavelength-dependent instrument response from the measurement.



Typical Relative Irradiance Setup

Common applications include characterizing the light output of LEDs, incandescent lamps, and other radiant energy sources such as sunlight. Relative irradiance measurements also include fluorescence measurements, which measure the energy given off by materials that have been excited by light at shorter wavelengths.

### ► Procedure

Perform the following steps to take a relative irradiance measurement using SpectraSuite:

1. Place SpectraSuite in Scope mode by clicking the Scope () icon in the Experiment mode toolbar or selecting **Processing | Processing Mode | Scope** from the menu.
2. Ensure that the entire signal is on scale. The intensity of the reference signal should peak at about 50000 counts. If necessary, adjust the integration time until the intensity is approximately 50000 counts.
3. Take a reference spectrum using a light source with a black body of a known color temperature, such as the LS-1.
4. Click the Store Reference Spectrum () icon on the toolbar or by select **File | Store | Store Reference Spectrum** from the menu bar to store the reference. This command merely stores a reference spectrum in memory. You must click the Save Spectra () icon on the toolbar or select **File | Save | Save Spectra Collection** from the menu bar to permanently save the reference spectrum to disk.
5. If you have not already done so, store a dark spectrum reading. To do this, either block the light path to the spectrometer, uncheck the **Strobe/Lamp Enable** box in the Acquisition toolbar, or turn the light source off. Then, take a dark spectrum by clicking the Store Dark Spectrum () icon on the toolbar or by selecting **File | Store | Store Dark Spectrum** from the menu bar. This command merely stores a dark spectrum in memory. You must click the Save Spectra () icon on the toolbar.

---

### Note

If possible, do not turn off the light source when taking a dark spectrum. If you must turn off your light source to store a dark spectrum, allow enough time for the lamp to warm up again before continuing your experiment.

---

You must take a dark spectrum before measuring relative irradiance.

6. Position the fiber at the light source you want to measure. Then, click . The Relative Irradiance graph appears.

---

## Appendix A

# Calibrating the Wavelength of the USB4000

## Overview

This appendix describes how to calibrate the wavelength of your spectrometer. Though each spectrometer is calibrated before it leaves Ocean Optics, the wavelength for all spectrometers will drift slightly as a function of time and environmental conditions. Ocean Optics recommends periodically recalibrating the USB4000.

## About Wavelength Calibration

You are going to be solving the following equation, which shows that the relationship between pixel number and wavelength is a third-order polynomial:

$$\lambda_p = I + C_1 p + C_2 p^2 + C_3 p^3$$

Where:

$\lambda$  = the wavelength of pixel  $p$

$I$  = the wavelength of pixel 0

$C_1$  = the first coefficient (nm/pixel)

$C_2$  = the second coefficient (nm/pixel<sup>2</sup>)

$C_3$  = the third coefficient (nm/pixel<sup>3</sup>)

$R_\lambda$  = the reference intensity at wavelength  $\lambda$

You will be calculating the value for  $I$  and the three  $C$ s.

# Calibrating the Spectrometer

## Preparing for Calibration

To recalibrate the wavelength of your spectrometer, you need the following components:

- A light source capable of producing spectral lines

---

### Note

Ocean Optics' HG-1 Mercury-Argon lamp is ideal for recalibration. If you do not have an HG-1, you need a light source that produces several (at least 4-6) spectral lines in the wavelength region of your spectrometer.

- 
- An USB4000 spectrometer
  - An optical fiber (for spectrometers without a built-in slit, a 50- $\mu\text{m}$  fiber works best)
  - A spreadsheet program (Excel or Quattro Pro, for example) or a calculator that performs third-order linear regressions

---

### Note

If you are using Microsoft Excel, choose **Tools | Add-Ins** and check **AnalysisToolPak** and **AnalysisToolPak-VBA**.

## Calibrating the Wavelength of the Spectrometer

### ► Procedure

Perform the steps below to calibrate the wavelength of the spectrometer:

1. Place SpectraSuite into Scope mode and take a spectrum of your light source. Adjust the integration time (or the A/D conversion frequency) until there are several peaks on the screen that are not off-scale.
2. Move the cursor to one of the peaks and position the cursor so that it is at the point of maximum intensity.
3. Record the pixel number that is displayed in the status bar or legend (located beneath the graph). Repeat this step for all of the peaks in your spectrum.
4. Use the spreadsheet program or calculator to create a table like the one shown in the following figure. In the first column, place the exact or true wavelength of the spectral lines that you used. In the second column of this worksheet, place the observed pixel number. In the third column, calculate the pixel number squared, and in the fourth column, calculate the pixel number cubed.

Independent Variable	Dependent Variables			Values Computed from the Regression Output	
True Wavelength (nm)	Pixel #	Pixel # <sup>2</sup>	Pixel # <sup>3</sup>	Predicted Wavelength	Difference
253.65	175	30625	5359375	253.56	0.09
296.73	296	87616	25934336	296.72	0.01
302.15	312	97344	30371328	302.40	-0.25
313.16	342	116964	40001688	313.02	0.13
334.15	402	161604	64964808	334.19	-0.05
365.02	490	240100	117649000	365.05	-0.04
404.66	604	364816	220348864	404.67	-0.01
407.78	613	375769	230346397	407.78	0.00
435.84	694	481636	334255384	435.65	0.19
546.07	1022	1044484	1067462648	546.13	-0.06
576.96	1116	1245456	1389928896	577.05	-0.09
579.07	1122	1258884	1412467848	579.01	0.06
696.54	1491	2223081	3314613771	696.70	-0.15
706.72	1523	2319529	3532642667	706.62	0.10
727.29	1590	2528100	4019679000	727.24	0.06
738.40	1627	2647129	4306878883	738.53	-0.13
751.47	1669	2785561	4649101309	751.27	0.19

- Use the spreadsheet or calculator to calculate the wavelength calibration coefficients. In the spreadsheet program, find the functions to perform linear regressions.
  - If using Quattro Pro, look under **Tools | Advanced Math**
  - If using Excel, look under **Analysis ToolPak**
- Select the true wavelength as the dependent variable (Y). Select the pixel number, pixel number squared, and the pixel number cubed as the independent variables (X). After executing the regression, you will obtain an output similar to the one shown below. Numbers of importance are noted.

**Regression Statistics**

Multiple R      0.999999831  
 R Square        0.999999663 ← R Squared  
 Adjusted R Square 0.999999607  
 Standard Error 0.125540214  
 Observations   22

	<b><u>Coefficients</u></b>	<b><u>Standard Error</u></b>	
Intercept	190.473993	0.369047536	← First coefficient
X Variable 1	0.36263983	0.001684745	← Second coefficient
X Variable 2	-1.174416E-05	8.35279E-07	
X Variable 3	-2.523787E-09	2.656608E-10	← Third coefficient

- Record the Intercept, as well as the First, Second, and Third Coefficients. Additionally, look at the value for R squared. It should be very close to 1. If not, you have most likely assigned one of your wavelengths incorrectly.

Keep these values at hand.

## Saving the New Calibration Coefficients: USB Mode

Ocean Optics programs wavelength calibration coefficients unique to each USB4000 onto an EEPROM memory chip in the USB4000.

You can overwrite old calibration coefficients on the EEPROM if you are using the USB4000 via the USB port.

### ► Procedure

To save wavelength calibration coefficients using the USB mode, perform the following steps:

- Ensure that the USB4000 is connected to the computer and that you have closed all other applications.
- Point your browser to <http://www.oceanoptics.com/technical/softwaredownloads.asp> and scroll down to **Microcode**. Select **USB EEPROM Programmer**.
- Save the setup file to your computer.
- Run the **Setup.exe** file to install the software. The **Welcome** screen appears.
- Click the **Next** button. The **Destination Location** screen appears.
- Accept the default installation location, or click the **Browse** button to specify a directory. Then, click the **Next** button. The **Program Manager Group** screen appears.
- Click the **Next** button. The **Start Installation** screen appears.
- Click the **Next** button to begin the installation. Once the installation finishes, the **Installation Complete** screen appears.
- Click the **Finish** button and reboot the computer when prompted.
- Navigate to the **USB EEPROM Programmer** from the Start menu and run the software.
- Click on the desired USB4000 device displayed in the left pane of the **USB Programmer** screen.
- Double-click on each of the calibration coefficients displayed in the right pane of the USB Programmer screen and enter the new values acquired in Steps 5 and 6 of the [Calibrating the Wavelength of the Spectrometer](#) section in this appendix.
- Repeat Step 12 for all of the new values.
- Click on the **Save All Values** button to save the information, and then **Exit** the USB Programmer software.

The new wavelength calibration coefficients are now loaded onto the EEPROM memory chip on the USB4000.

# External Triggering

## Overview

The USB4000 supports five triggering modes, which are set with the Trigger Mode command. A detail of each triggering mode follows.

### Normal (Free Running)

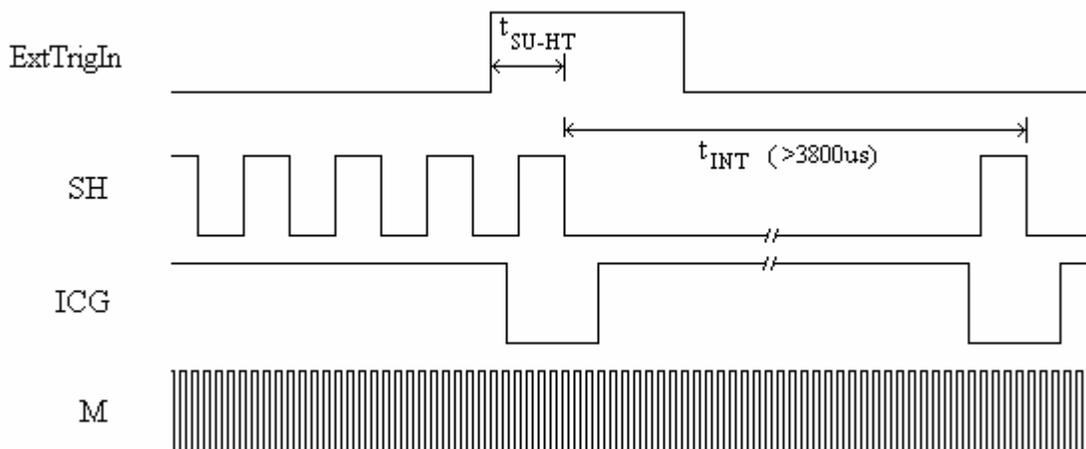
In this mode, the USB4000 uses the user-defined integration clock and continuously scans the CCD array. All of the signals described in the previous section are provided by the spectrometer to the CCD automatically based on the integration time selected in the software by the user.

### External Software Trigger

In this mode, the ExtTrigIn signal acts as an enable switch. If ExtTrigIn is kept HIGH, the USB4000 will acquire spectra as if it was in the normal free running mode. If ExtTrigIn is kept LOW, the USB4000 will not acquire spectra.

### External Hardware Trigger

In this mode, the USB4000 uses the software (user) defined integration clock; however, the integration period doesn't begin until the External Trigger Input Signal (ExtTrigIn) goes HIGH. If no External Trigger Input Signal is applied, the spectrometer will not take any spectra, and the software will appear "frozen" until an External Trigger Input Signal is detected. With ExtTrigIn going HIGH, the spectrometer will provide the required signals to the CCD as shown below (note that in the following diagram, the spectrometer is in non-shutter mode):



**External Hardware Trigger Mode (non-shutter mode)**

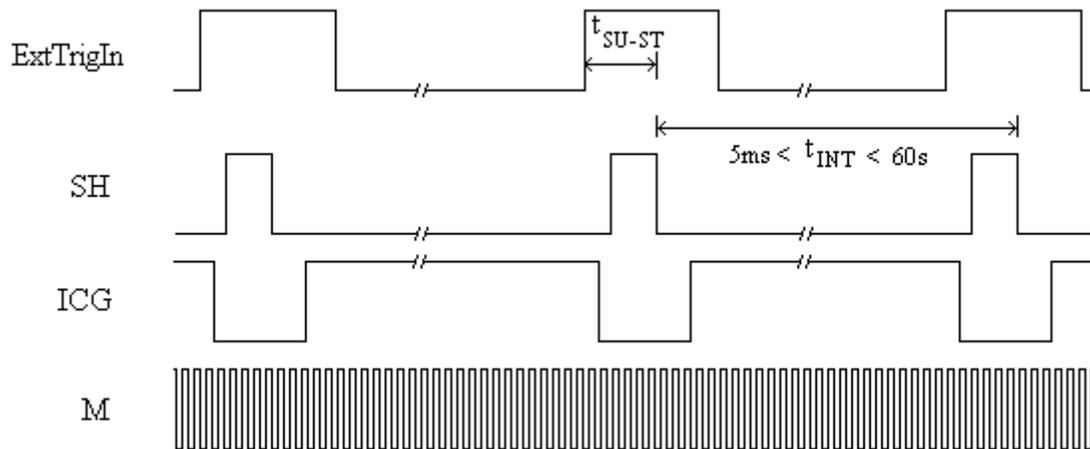
There is a small delay from when ExtTrigIn goes HIGH to when the integration period begins. This time is defined as  $t_{SU-HT}$ , and is specified to be between  $10\mu s$ - $12\mu s$ . Though the picture above shows the USB4000 in non-shutter mode ( $t_{INT} > 3800\mu s$ ), External Hardware Trigger Mode can run in shutter mode ( $t_{INT} < 3800\mu s$ ) as well (in this case, the SH signal will continue to run after ICG as discussed earlier in the shutter mode section of this document). Regardless of whether the spectrometer is in shutter or non-shutter mode, SH continues to run while waiting for ExtTrigIn in order to keep the detector from acquiring spectral data.

**External Hardware Trigger Delay**

The delay between the rising edge of ExtTrigIn and the beginning of the integration period can be extended through the External Hardware Trigger Delay feature accessible through the software user interface. The External Hardware Trigger Delay is adjustable in 500ns increments. The actual delay is the value set by the External Hardware Trigger Delay plus  $t_{SU-HT}$  ( $10\mu s$ - $12\mu s$ ). So, for example, if the Hardware Trigger Delay is set to  $65\mu s$ , the integration period will begin  $75\mu s$ - $77\mu s$  after ExtTrigIn goes HIGH.

**External Synchronization Trigger**

In this mode of the USB4000, the integration clock is essentially input into the spectrometer. The synchronized trigger must have a frequency range of 5ms to 60s (shutter mode cannot be used in External Synchronization Trigger mode). If no External Trigger Input Signal is applied, the spectrometer will not take any spectra, and the software will appear “frozen” until an External Trigger Input Signal is detected. With a continuous ExtTrigIn, the spectrometer will provide the required signals to the CCD as shown below:



### External Synchronization Trigger

The time between when ExtTrigIn goes HIGH and the beginning of the integration period is specified to be between  $8\mu s < t_{SU-ST} < 10\mu s$ . The ExtTrigIn signal does not need to have an even duty cycle, but the time between rising edges should remain constant for a given integration time.

## Quasi-Real Time Acquisition Mode

While this is classified as a trigger mode, it's important to realize that no trigger signal is required to operate in this mode. In this mode, the integration clock is set to 4ms, which is the time required to completely read out all the pixels. When the software (user) requests a spectrum, the integration clock waits for the current period to expire, changes to the desired integration time set via software commands, and then returns to 4ms. With this approach, the start of the integration period will always be within 4ms of the time when the request for a spectrum is issued.

## B: External Triggering

---

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# Appendix C

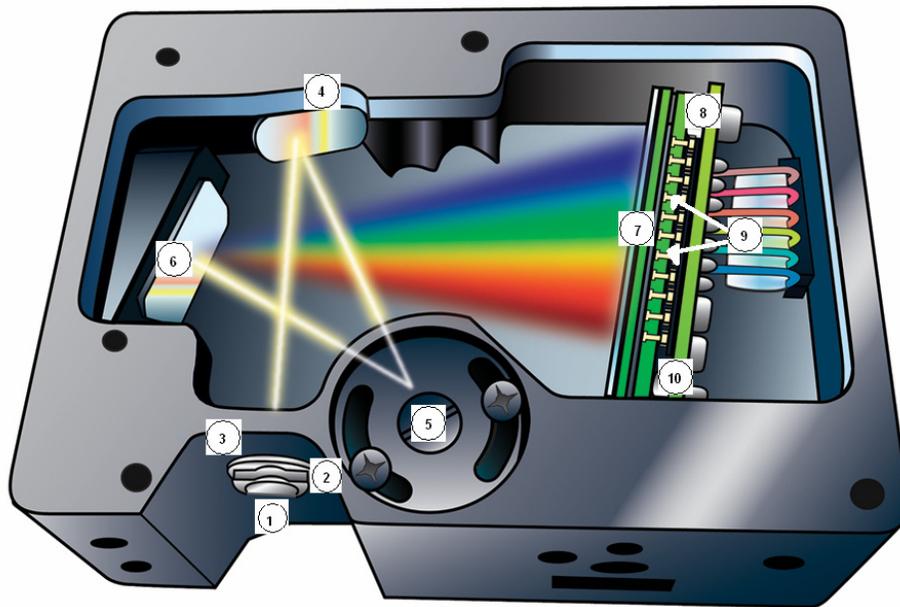
# Specifications

## Overview

This appendix contains information on spectrometer operation, specifications, and system compatibility. It also includes accessory connector pinout diagrams and pin-specific information.

## How the USB4000 Works

Below is a diagram of how light moves through the optical bench of an USB4000 Spectrometer. The optical bench has no moving parts that can wear or break; all the components are fixed in place at the time of manufacture. Items with an asterisk (\*) are user-specified.



**USB4000 Spectrometer with Components**

See [USB4000 Components Table](#) on the following page for an explanation of the function of each numbered component in the USB4000 Spectrometer in this diagram.

## USB4000 Components Table

Ocean Optics permanently secures all components in the USB4000 at the time of manufacture. Only Ocean Optics technicians can replace interchangeable components, where noted.

Item	Name	Description
1	SMA 905 Connector	Secures the input fiber to the spectrometer. Light from the input fiber enters the optical bench through this connector.
2	Slit	<p>A dark piece of material containing a rectangular aperture, which is mounted directly behind the SMA Connector. The size of the aperture (from 5 <math>\mu\text{m}</math> to 200 <math>\mu\text{m}</math>) regulates the amount of light that enters the optical bench and controls spectral resolution.</p> <p>You can also use the USB4000 without a Slit. In this configuration, the diameter of the fiber connected to the USB4000 determines the size of the entrance aperture.</p> <p>Only Ocean Optics technicians can change the Slit.</p>
3	Filter	<p>Restricts optical radiation to pre-determined wavelength regions. Light passes through the Filter before entering the optical bench. Both bandpass and longpass filters are available to restrict radiation to certain wavelength regions.</p> <p>Only Ocean Optics technicians can change the Filter.</p>
4	Collimating Mirror	<p>Focuses light entering the optical bench towards the Grating of the spectrometer. Specify standard or SAG+.</p> <p>Light enters the spectrometer, passes through the SMA Connector, Slit, and Filter, and then reflects off the Collimating Mirror onto the Grating.</p>
5	Grating	<p>Diffraction light from the Collimating Mirror and directs the diffracted light onto the Focusing Mirror. Gratings are available in different groove densities, allowing you to specify wavelength coverage and resolution in the spectrometer.</p> <p>Only Ocean Optics technicians can change the Grating.</p>
6	Focusing Mirror	Receives light reflected from the Grating and focuses first-order spectra onto the detector plane.
7	L4 Detector Collection Lens	<p>An optional component that attaches to the Detector to increase light-collection efficiency. It focuses light from a tall slit onto the shorter Detector elements.</p> <p>The L4 Detector Collection Lens should be used with large diameter slits or in applications with low light levels. It also improves efficiency by reducing the effects of stray light.</p> <p>Only Ocean Optics technicians can add or remove the L4 Detection Collection Lens.</p>
8	Detector (UV or VIS)	Collects the light received from the Focusing Mirror or L4 Detector Collection Lens and converts the optical signal to a digital signal. Each pixel on the Detector responds to the wavelength of light that strikes it, creating a digital response. The spectrometer then transmits the digital signal to the SpectraSuite application.

Item	Name	Description
9	OFLV Filters	OFLV Variable Longpass Order-sorting Filters block second- and third-order light. These filters are optional.
10	UV4 Detector Upgrade	The detector's standard window is replaced with a quartz window to enhance spectrometer performance (<340 nm). This upgrade is optional.

## USB4000 Specifications

The following sections provide specification information for the CCD detector in the USB4000, as well as the USB4000 Spectrometer itself.

### CCD Detector Specifications

Specification	Value
Detector	Toshiba TCD1304AP linear CCD array
No. of elements	3648 pixels
Sensitivity	130 photons per count at 400 nm; 60 photons/count at 600 nm
Pixel size	8 $\mu\text{m}$ x 200 $\mu\text{m}$
Pixel well depth	~100,000 electrons
Signal-to-noise ratio	300:1 (at full signal)
A/D resolution	16 bit
Dark noise	50 RMS counts
Corrected linearity	>99.8%

### USB4000 Spectrometer

Specification	Value
Dimensions	89.1 mm x 63.3 mm x 34.4 mm
Weight	190 g
Power consumption	250 mA @ 5 VDC

## C: Specifications

Specification	Value
Detector	3648-element linear silicon CCD array
Detector range	200-1100 nm
Gratings	14 gratings available
Entrance aperture	5, 10, 25, 50, 100 or 200 $\mu$ m wide slits
Order-sorting filters	Installed longpass and bandpass filters
Focal length	42 mm input; 68 mm output
Optical resolution	Depends on grating and size of entrance aperture
Stray light	<0.05% at 600 nm; <0.10% at 435 nm
Dynamic range	$2 \times 10^8$ (system); 1300:1 for a single acquisition
Fiber optic connector	SMA 905 to single-strand optical fiber (0.22 NA)
Data transfer rate	Full scans into memory every 4 milliseconds with USB 2.0 port
Integration time	10 microseconds to >60 seconds (detector's limit is ~15 sec)
Interfaces	USB 2.0, 480 Mbps (USB 1.1 compatible); RS-232 (2-wire) @ 115.2 K baud
Operating systems	Windows 98/Me/2000/XP, Mac OS X, and Linux when using the USB port. Any 32-bit Windows operating system when using the serial port.
Onboard GPIO	10 user-programmable digital I/Os
Analog channels	No

# 22-Pin Accessory Connector Pinout

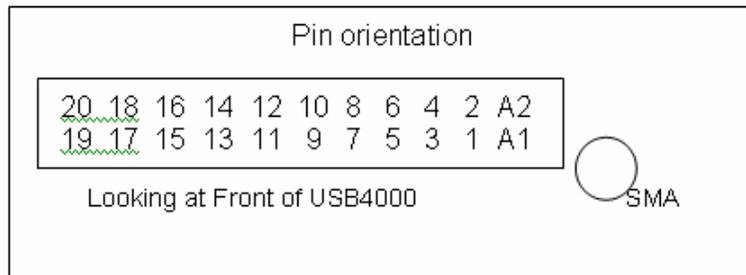
The USB4000 features a 22-pin Accessory Connector, located on the front of the unit as shown:



Location of USB4000 22-Pin Accessory Connector

## 22-Pin Accessory Connector Pinout Diagram

When facing the 22-pin Accessory Connector on the front of the vertical wall of the USB4000, pin numbering is as follows:



22-Pin Accessory Connector Pinout Diagram

## 22-Pin Accessory Connector – Pin Definitions and Descriptions

The following table contains information regarding the function of each pin in the USB4000's 22-Pin Accessory Connector:

Pin #	Function	Input/Output	Description
1	V <sub>CC</sub> , V <sub>USB</sub> , or 5V <sub>IN</sub>	Input or Output	Input power pin for USB4000 – When operating via USB, this pin can power other peripherals – Ensure that peripherals comply with USB specifications
2	RS232 Tx	Output	RS232 transmit signal – Communicates with a computer over DB9 Pin 2
3	RS232 Rx	Input	RS232 receive signal – Communicates with a computer over DB9 Pin 3
4	Lamp Enable	Output	TTL signal driven Active HIGH when the Lamp Enable command is sent to the spectrometer
5	Continuous Strobe	Output	TTL output signal used to pulse a strobe – Divided down from the master clock signal
6	Ground	Input/Output	Ground
7	External Trigger In	Input	TTL input trigger signal – See External Triggering Options document for info
8	Single Strobe	Output	TTL output pulse used as a strobe signal – Has a programmable delay relative to the beginning of the spectrometer integration period
9	I <sup>2</sup> C SCL	Input/Output	The I <sup>2</sup> C clock signal for communications to other I <sup>2</sup> C peripherals.
10	I <sup>2</sup> C SDA	Input/Output	The I <sup>2</sup> C Data signal for communications to other I <sup>2</sup> C peripherals.
11	MOSI	Output	SPI Master Out Slave In (MOSI) signal for communication to other SPI peripherals
12	MISO	Input	SPI Master In Slave Out (MISO) signal for communication to other SPI peripherals
13	GPIO-1	Input/Output	General purpose software-programmable, digital input/output (channel number)
14	GPIO-2	Input/Output	General purpose software-programmable, digital input/output (channel number)

Pin #	Function	Input/Output	Description
15	GPIO-1	Input/Output	General purpose software-programmable, digital input/output (channel number)
16	GPIO-2	Input/Output	General purpose software-programmable, digital input/output (channel number)
17	GPIO-3	Input/Output	General purpose software-programmable, digital input/output (channel number)
18	GPIO-4	Input/Output	General purpose software-programmable, digital input/output (channel number)
19	GPIO-3	Input/Output	General purpose software-programmable, digital input/output (channel number)
20	GPIO-4	Input/Output	General purpose software-programmable, digital input/output (channel number)
A1	SPI_CLK	Output	SPI clock signal for communication to other SPI peripherals
A2	SPICS OUT	Output	The SPI Chip/Device Select signal for communications to other SPI peripherals

## 22-Pin Accessory Connector - Part Numbers

The part numbers for the 22-pin accessory connector on the USB4000 Spectrometer are as follows:

- The connector is a Samtec Part Number **IPT1-111-01-S-D-RA**.
- The vertical mating connector is Part Number **IPS1-111-01-S-D-VS**.
- The right-angle PCB mount is Part Number **IPS1-111-01-S-D-RA**.

If you are customizing your USB4000 Spectrometer system or configuring External Triggering, you may need these part numbers to complete your setup.



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