NIRQuest
Installation and Operation Manual

For Products: NIRQuest512-1.7, NIRQuest512-1.9, NIRQuest512-2.2, NIRQuest512-2.5, NIRQuest256-2.1, NIRQuest256-2.5

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About This Manual

Document Purpose and Intended Audience

This document provides you with instructions to get your system up and running. In addition to the NIRQuest Spectrometer installation and operation instructions, this manual also includes information for locating the OceanView software instructions

What's New in this Document

This version of the *NIRQuest Near Infrared Fiber Optics Spectrometers Installation and Operation Manual* updates for the Kensington® security slot.

Document Summary

Chapter	Description
Chapter 1: *Introduction*	Introduces the product features. Also contains a list of items included in the shipment.
Chapter 2: *Installing the NIRQuest Spectrometer*	Contains information for installing and configuring your NIRQuest Spectrometer. These instructions include information on using your NIRQuest Spectrometer with the spectrometer operating software.
Chapter 3: *Troubleshooting*	Contains typical problems and suggested resolutions.
Appendix A: *Calibrating the Wavelength of the NIRQuest Spectrometer*	Contains instructions for calibrating your NIRQuest Spectrometer.
Appendix B: *Specifications*	Contains technical specifications for the NIRQuest Spectrometer and the NIR Detector. It also includes grating efficiency graphs and pinout information.
Appendix C: *NIRQuest512-2.5 and NIRQuest256-2.5 Sensitivity*	Provides some additional sensitivity specifications for the NIRQuest256-2.5 and NIRQuest512-2.5 Spectrometer.

Product-Related Documentation

Document for…	Document Location
OceanView software	http://oceanoptics.com/wp-content/uploads/OceanViewIO.pdf
HR-4 Breakout Box	http://oceanoptics.com/wp-content/uploads/HR-4-Breakout-Box.pdf
External triggering	http://oceanoptics.com/wp-content/uploads/External-Triggering-Options_Firmware3.0andAbove.pdf
Device driver issues	http://oceanoptics.com/wp-content/uploads/Correcting-Device-Driver-Issues.pdf

Ocean Optics offers a Glossary of spectroscopy terms to help you further understand your state-of-the-art products and how they function, located at: **http://oceanoptics.com/glossary/.**

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.

Warranty

Our 3-Year Warranty covers Ocean Optics miniature fiber optic spectrometers, light sources and sampling accessories – regardless of the application – from manufacturing defects. It also covers fibers and probes for a full 12 months: **http://www.oceanoptics.com/warranty.asp**

This comprehensive warranty ensures you of the highest level of craftsmanship and reliability for years to come. No other manufacturer offers such a solid guarantee of quality and reliability.

The Ocean Optics 3-Year Warranty applies to Ocean Optics equipment (excluding OEM configurations) purchased on or after July 1, 2010. The warranty covers parts and labor needed to repair manufacturing defects that occur during the warranty period. We also will cover the costs of shipping warranty-related repairs from our customers to Ocean Optics and from us to our customers.

ISO Certification

Ocean Optics, the industry leader in miniature photonics, has been certified for ISO 9001:2008 certification applicable to the design and manufacture of electro-optical equipment since 2009.

WARNING

This is a Class A product. In a domestic environment this product may cause radio interference in which case the user may be required to take adequate measures.

FCC COMPLIANCE

This equipment has been tested and found to comply with the limits for a Class A digital device, pursuant to Part 15 of the FCC Rules. These limits are designed to provide reasonable protection against harmful interference when the equipment is operated in a commercial environment. This equipment generates, uses and can radiate radio frequency energy and, if not installed and used in accordance with the instruction manual, may cause harmful interference to radio communications. Operation of this equipment in a residential area is likely to cause harmful interference in which the user will be required to correct the interference at his on expense.

WARNING: The authority to operate this equipment is conditioned by the requirement that no modifications will be made to the equipment unless the changes or modifications are expressly approved by the manufacturer.

Chapter 1

Introduction

Product Description

A high-performance optical bench, low-noise electronics and various grating options make NIRQuest Spectrometers the best choice for modular NIR spectroscopy. This small footprint, near infrared spectrometer is available in several different models that cover various wavelength ranges between 900 nm and 2500 nm and as with most Ocean Optics designs can be customized for your specific application with various grating, slit and mirror options. The NIRquest is ideal for applications ranging from analyzing moisture content in food and beverage products to analyzing trace metals in wastewater and laser characterization, among others.

Note

High Gain Mode is not recommended for NIRQuest512-2.2 and NIRQuest512-2.5 spectrometers, but can be used. An additional 30 minute warm-up time is necessary to stabilize the detector response.

The NIRQuest (Near Infrared) Fiber Optic Spectrometer combines the high-performance InGaAs array detector with the high-sensitivity NIRQuest optical bench. The NIRQuest Spectrometer and the 16-bit A/D converter share a single housing, forming a small-footprint plug-and-play system.

The NIRquest communicates via the Universal Serial Bus (USB) connection with an external 5V power source. A 30-pin interface provides several GPIO ports. The optional high gain mode can be used for those applications requiring extra sensitivity.

An optional internal shutter is available on custom-configured spectrometers (INTERNAL-SHUTTER-LRG-BENCH). This makes it easier to take dark measurements and when you need fast integration times with the best possible signal. This optional feature is also recommended for probe-based or emissive measurements where it is difficult to introduce a shutter into the optical path. The shutter can be added to an existing NIRQuest for an extra charge.

Replaceable slits are offered for added convenience. Deep UV option includes purge port.

About the Modular Approach

Ocean Optics fiber optic spectrometer systems are based on low-cost, modular data acquisition principles. A typical NIRQuest Spectrometer system contains four basic elements:

- The NIRQuest Spectrometer (see *NIRQuest Spectrometer Models*)
- The Ocean Optics OceanView spectrometer operating software (see *Product-Related Documentation*)
- A light (excitation source) (see *Accessories*)
- A variety of sampling optics (depending on application need) (see *Accessories*)

The light (excitation source) sends light through an optical fiber to the sample. The light interacts with the sample, and the results are collected and transmitted through another optical fiber to the spectrometer. The spectrometer measures the amount of light and transforms the data collected by the spectrometer into digital information. Finally, the spectrometer passes that information to the operating software.

NIRQuest Spectrometer Models

The NIRQuest family of spectrometers consists of the following models:

- NIRQuest512-1.7 with a detector range of 850 – 1700 nm; usable range of 900 – 2700 nm
- NIRQuest512-1.9 with a detector range of 1000 – 1900 nm; usable range 1100 – 1900 nm
- NIRQuest512-2.2 with a detector range 900 – 2200 nm; usable range of 900 – 2200 nm
- NIRQuest512-2.5 with a detector range 900 – 2550 nm; usable range of 900 – 2500 nm
- NIRQuest256-2.1 with a detector range of 900 – 2100 nm; usable range of 900 – 2050 nm
- NIRQuest256-2.5 with a detector range of 900 – 2550 nm; usable range of 900 – 2500 nm

About OceanView Software

OceanView is the latest generation of operating software for all Ocean Optics spectrometers. It 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.

OceanView is a user-customizable, advanced acquisition and display program that provides a real-time interface to a variety of signal-processing functions. With OceanView, 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. Consult the OceanView manual for hardware requirements when using OceanView (see

Accessories

Ocean Optics also offers a complete line of spectroscopic accessories to use with the NIRQuest Spectrometer. Most spectroscopic accessories have SMA connectors for application flexibility. Thus, changing the sampling system is as easy as unscrewing a connector and adding a new component or accessory.

A partial list of Ocean Optics spectroscopic accessories includes light sources, sampling holders, filter holders, flow cells, fiber optic probes and sensors, collimating lenses, attenuators, diffuse reflectance standards, integrating spheres and an extensive line of optical fibers.

This modular approach, where components are easily mixed and matched, offers remarkable applications flexibility. You can select from hundreds of products to create distinctive systems for an almost endless variety of optical-sensing applications.

Breakout Box

Ocean Optics also offers the Breakout Box (HR4-BREAKOUT), a passive module that separates the signals from their 30-pin port to an array of standard connectors and headers, enabling easy access to a variety of features found in Ocean Optics' NIRQuest 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.

Features

- High signal-to-noise ratio: 15,000:1 to 7500:1, depending on model. Combined with high dynamic range this means that you can achieve the highest accuracy and precision, important for modeling.
- Deep TEC cooling down from 35°C to 50°C below ambient. This means lower dark current and improved signal to noise.
- High Resolution: 2nm - 12nm (slit and detector dependent) to suit your application.
- Small and lightweight: 182 x 110 x 47 mm and 1.2 kg.
- Configurable with a range of detectors, gratings and slits for your specific application.
- Rugged and proven diode array technology with no moving parts.
- Continuous real-time spectral data in the field, on the line or in the lab.
- Fast data transfer via USB and optional RS-232. GPIO pins support I2C peripherals.
- Access to Ocean Optics' unrivaled range of software, light sources, sampling and fiber accessories.
- Hamamatsu G9204-512 (NIRQuest512), G9205-512 (NIRQUEST512-1.9), G9206-512W (NIRQuest512-2.2), G9208-512W (NIRQuest512-2.5), G9206-256 (NIRQuest256-2.1), G9208-256 (NIRQuest256-2.5) InGaAs linear array detector
  - Wide dynamic range
  - Low noise and low dark current
- Spectrometer Design
  - Symmetrical Crossed Czerny Turner
  - 101mm focal length
  - 4 gratings (model-dependent)
  - 6 slit widths
  - Interchangeable slits
- Electrical Performance
  - 16 bit, 500KHz A/D converter
  - Integration times from 1 ms to 120 seconds (depending on spectrometer model)
- Embedded microcontroller allows programmatic control of all operating parameters and standalone operation
  - USB 2.0 480Mbps

  - Communication standards for digital accessories (I2C)
- Onboard Pulse Generator
  - 3 programmable strobe signals for triggering other devices
  - Software control of nearly all pulse parameters
- Onboard GPIO
  - 10 user-programmable digital I/Os
- EEPROM storage for
  - Wavelength Calibration Coefficients
  - Linearity Correction Coefficients
  - Absolute Irradiance Calibration (optional)
- Plug-n-play interface for PC applications
- 30-pin connector for interfacing to external products
- Kensington® security slot
- Optional shutter for dark measurements requiring a fast integration time and good throughput – Specify when ordering
- CE certification

Interface Options

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

Computer Interface	Operating System Requirements	Cable Needed	Description of Cable
Desktop or Notebook PC via USB Port	Windows Me/ 2000/XP	USB-CBL-1 (included)	Cable connects from USB port on NIRQuest Spectrometer to USB port on desktop or notebook PC
Desktop or Notebook PC via Serial Port	Any 32-bit Windows operating system	HR4-BREAKOUT (not included)	Adapter block that enables connection from serial port on NIRQuest to serial port on desktop or notebook PC; comes with 5 VDC power supply (required when connecting to serial port)

Items Included with Shipment

- ❑ NIRQuest Spectrometer
- ❑ + 5VDC power supply

Important information and documentation accompany your NIRQuest Spectrometer upon shipment. This includes:

- Packing List – The packing list is located inside a plastic bag attached to the outside of the shipment box (the invoice is mailed separately). The items listed on the packing slip include all of the components in the order, including customized items installed in the spectrometer, such as the slit. The packing list also includes important information, such as the shipping and billing addresses, as well as any components on back order.
- Wavelength Calibration Data Sheet – Each spectrometer is shipped with a Wavelength Calibration Data Sheet that contains information unique to your spectrometer. OceanView reads this calibration data from your spectrometer when it interfaces to a PC via the USB port.

Note

Please save the Wavelength Calibration Data Sheet for future reference.

- 5V power supply
- 15-Pin Accessory Cable (see *NIRQuest 15-Pin Accessory Cable Pinout*)

Other Accessories Available

Visit us at **www.OceanOptics.com** for a complete list of products available for all of your spectroscopy needs.

- **Interchangeable Slits**
- **Fibers**
- **Light Sources**
- **Integrated Sampling Systems**
- **Cuvettes**
- **Filter Holders**
- **Lithium Ion Battery Pack**
- **HR4-BREAKOUT Breakout Box**
- **Remora Wireless Spectral Server**

Breakout Box

Ocean Optics also offers the Breakout Box (HR4-BREAKOUT), a passive module that separates the signals from their 30-pin port to an array of standard connectors and headers, enabling easy access to a variety of features found in Ocean Optics' NIRQuest Spectrometers. 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.

Chapter 2

Installing the NIRQuest Spectrometer

Overview

You must install the operating software application prior to connecting the NIRQuest Spectrometer to the PC. The Ocean Optics spectrometer operating software installs the drivers required for NIRQuest Spectrometer installation. If you do not install the software first, the system will not properly recognize the NIRQuest Spectrometer.

If you have already connected the NIRQuest Spectrometer to the PC prior to installing the software, consult Chapter 3: *Troubleshooting* for information on correcting a corrupt NIRQuest Spectrometer installation.

Once you have properly installed the spectrometer, refer to either the spectrometer operating instructions for information on taking measurements.

NIRQuest Spectrometer Installation

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

Caution

Ensure that TEC power is always applied (using OceanView software) before USB power.

USB Mode

Follow the steps in this section to interface the NIRQuest Spectrometer via the USB port to a desktop or notebook PC.

To connect the NIRQuest Spectrometer to a PC via the USB port, the PC must be running the Windows operating system.

► ***Procedure***

1. Install spectrometer operating software on the destination computer, and then reboot the system.

2. Plug the +5VDC wall adapter into an electrical outlet, then connect the power cord to the 2.5 mm power jack (older versions may have a 1.3 mm power jack) on the rear of the NIRQuest Spectrometer.
3. Locate the USB cable (USB-CBL-1) that came with the NIRQuest Spectrometer.
4. Insert the square end of the cable into the rear of the NIRQuest Spectrometer, and then insert the rectangular end into the USB port of the computer.

If the software was installed prior to connecting the NIRQuest Spectrometer, the **Add New Hardware Wizard** appears and installs the NIRQuest Spectrometer drivers. If the drivers do not successfully install, or if you connected the NIRQuest Spectrometer to the computer before installing the software, consult Chapter 4: *Troubleshooting*.

Note

Windows XP users may encounter a **Hardware Installation** warning window regarding Windows XP driver testing. Click the **Continue Installation** button at this screen, as this is an expected warning.

Serial Port Mode

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

► *Procedure*

Follow the steps below to connect the NIRQuest Spectrometer to the PC via serial port:

1. Plug the +5VDC wall adapter into an electrical outlet, then connect the power cord to the 2.5 mm power jack (older versions may have a 1.3 mm power jack) on the rear of the NIRQuest Spectrometer.
2. Connect one end of the serial cable to the RS-232 connector on the rear of the NIRQuest Spectrometer, and then connect the other end to a serial port on the PC.
3. Note the serial port number (also called COM Port) on the PC to which the NIRQuest Spectrometer is connected (some PCs may not have numbered ports).

The NIRQuest Spectrometer is now connected to the PC's serial port.

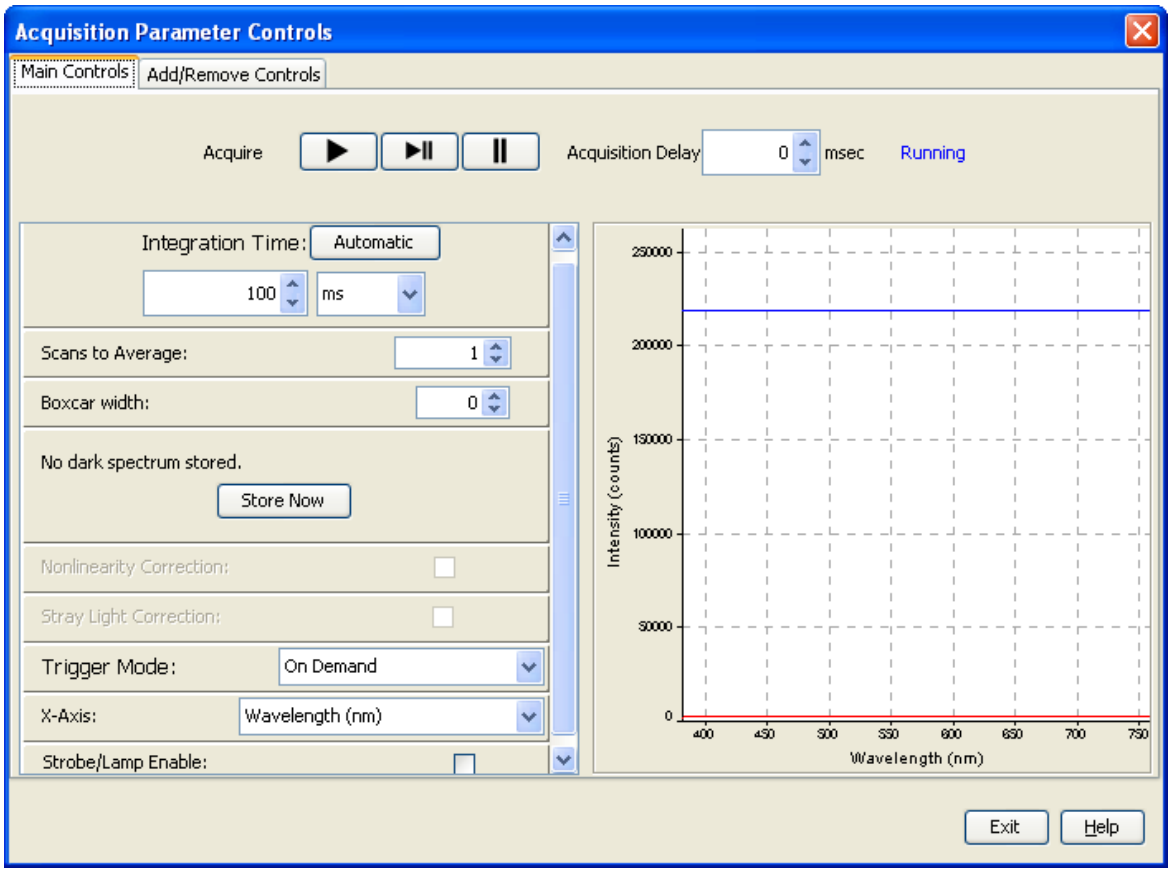
Configuring the NIRQuest Spectrometer

If you have followed the previous steps for connecting NIRQuest in USB mode and started OceanView, 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.

OceanView Acquisition Controls

In OceanView, the Acquisition Parameter Controls allow you to set the desired parameters for the NIRQuest.

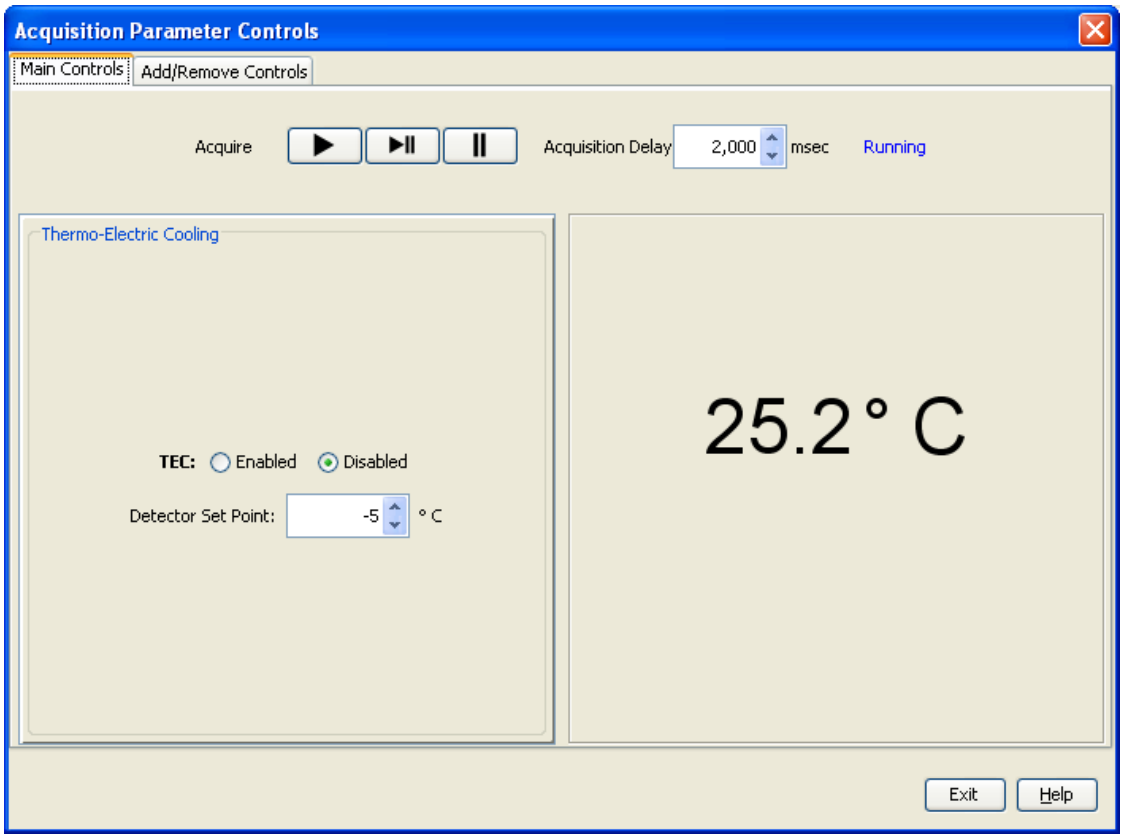


TE Cooler

► *Procedure*

To control the TE Cooler,

1. Right-click on the NIRQuest in the Schematic View.
2. Select New Acquisition | Thermo-Electric Cooling.

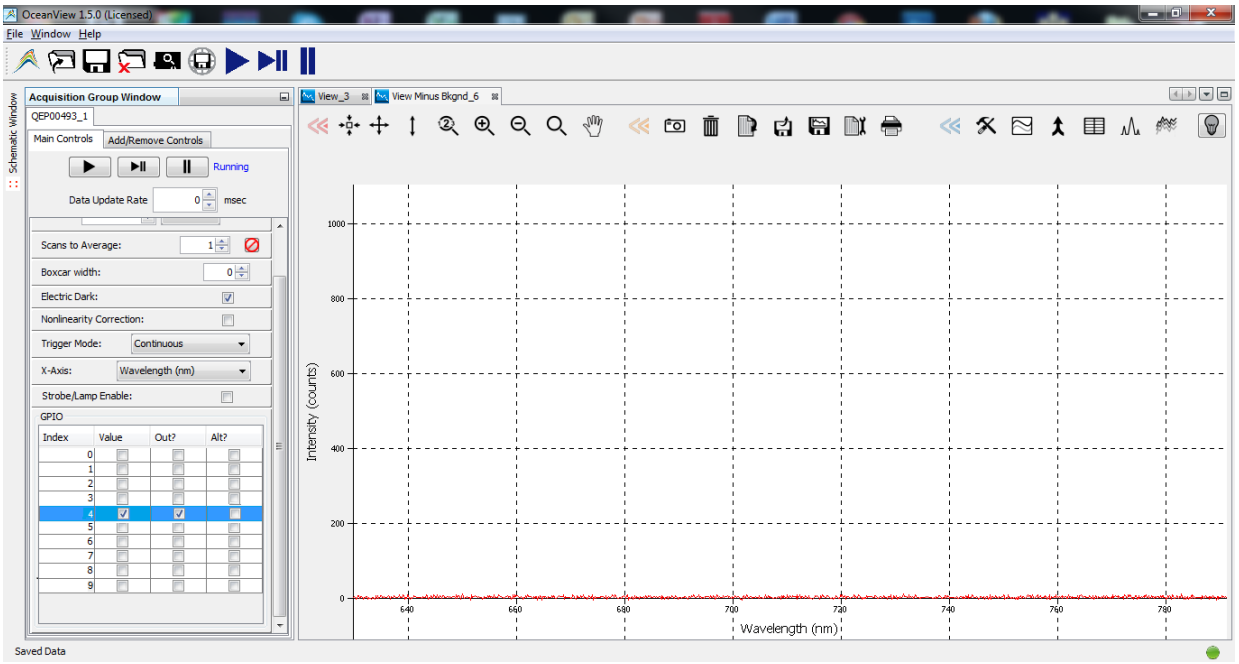


Optional Shutter

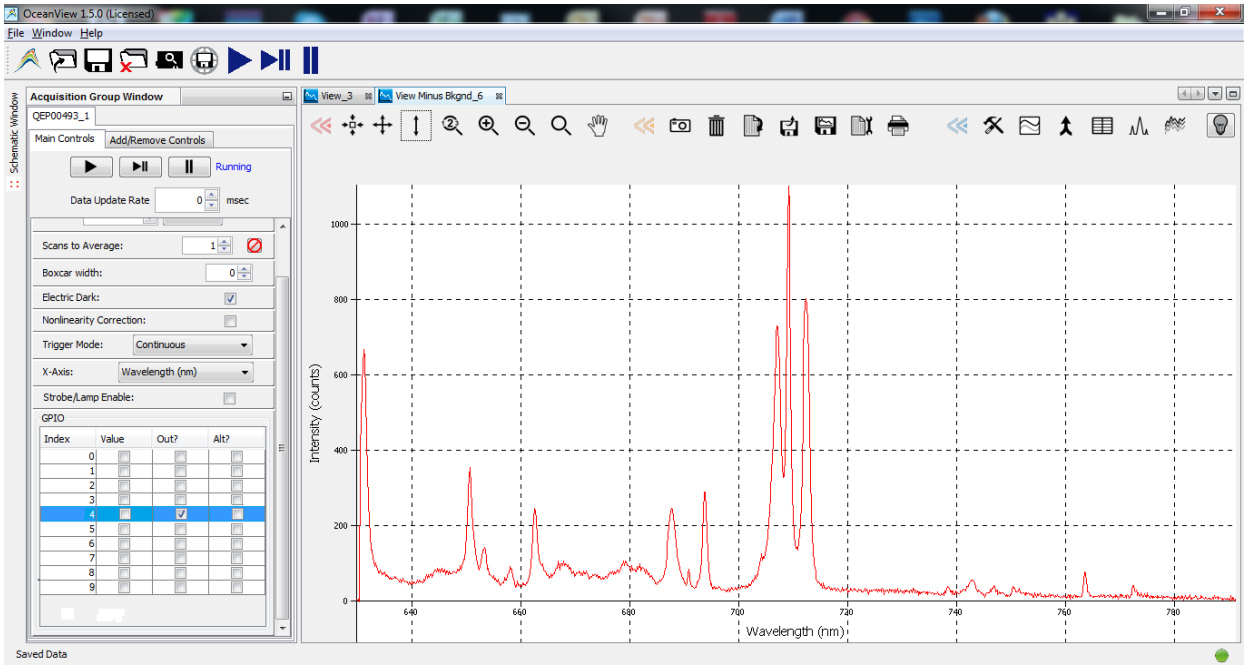
► *Procedure*

To enable the optional shutter,

1. In the Acquisition Group window, click on the **Add/Remove Controls** tab.
2. Select **GPIO**. The GPIO controls appear on the Main Controls tab.
3. Check the **Out** box for Index 4. This makes the GPIO an output.
4. Check the **Value** box for Index 4 to close the shutter. You can now take your dark measurement.



5. Uncheck the **Value** box to open the shutter.



Notes

Make sure the ALT checkbox for the GPIO (Index 4) is not selected, which would prevent the shutter from triggering.

The activation time of the internal shutter is 11 ms.

Connect Spectroscopic Accessories

To find operating instructions on NIRQuest Spectrometer-compatible products such as light sources, sampling chambers, probes, fibers or any other Ocean Optics spectroscopic accessories, check the the Ocean Optics website at:

http://oceanoptics.com/support/technical-documents/

Chapter 1: *Introduction* contains a list of NIRQuest Spectrometer-compatible products. You can find information related to these products on **http://www.oceanoptics.com/**.

External Triggering Options

You can trigger the NIRQuest Spectrometer using the External Software Triggering option through the 30-pin accessory connector on the spectrometer. Only the External Software Trigger mode is available with the NIRQuest Spectrometer.

The External Triggering Options document contains instructions on configuring External Triggering with the NIRQuest Spectrometer (see

Product-Related Documentation).

Change the Slit

There's no need to calibrate your spectrometer when changing the slit, just install and start measuring. There is one exception to this. You cannot change from a standard slit to a slit with a filter because it changes the optical focus and wavelength calibration of the spectrometer. In this case you would need to send the spectrometer back to Ocean Optics. A filter must be ordered for each slit (if your application requires a filter) and the spectrometer needs to be calibrated and focused with the filter installed. This only applies to filters installed inside the slit assembly.

► *Procedure*

1. Find the SMA connector. If a fiber is attached, remove it.

2. Use the Allen key to remove the 2 the screws attaching the slit to the spectrometer.
3. Pull the slit out of the spectrometer.
4. Put the new INTSMA slit connector into the spectrometer; with the key of the connector on the left side.

5. Install the 2 screws again. Use the Allen key to tighten the screws carefully (do not over-tighten).
6. If necessary, connect the fiber again.

Chapter 3

Troubleshooting

Overview

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

NIRQuest Spectrometer Connected to Computer Prior to Operating Software

Windows Operating Systems

If you connected your NIRQuest Spectrometer to the computer prior to installing your Ocean Optics software application, 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://oceanoptics.com///wp-content/uploads/Correcting-Device-Driver-Issues.pdf.**

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.

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.

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 NIRQuest Spectrometer from your computer.
6. Replug the spectrometer into your computer. The system should now be able to locate and install the correct drivers for the USB device.

Apple Mac OSX Operating Systems

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

Linux Operating Systems

For Linux operating systems, all you need to do is install the spectrometer operating 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.

Appendix A

Calibrating the Wavelength of the NIRQuest Spectrometer

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.

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:

λ = 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^2)

C_3 = the third coefficient (nm/pixel^3)

You will be calculating the value for I and the three Cs.

Calibrating the Spectrometer

Preparing for Calibration

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

- A light source capable of producing spectral lines.

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

If an order-sorting filter is installed in the NIRQuest, the XE-1 Xenon lamp is necessary to perform the wavelength calibration.

- The NIRQuest Spectrometer.
- An optical fiber (for spectrometers without a built-in slit, a 50-μm fiber works best).
- A spreadsheet program (Excel or Quattro Pro, for example) or a calculator that performs third-order linear regressions.
- If you are using Microsoft Excel, choose **Tools | Add-Ins** and check **AnalysisToolPak** and **AnalysisTookPak-VBA**.

Calibrating the Wavelength of the Spectrometer

► *Procedure*

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

1. Place spectrometer operating software into Quick View (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 # ^{2}	Pixel # ^{3}	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

5. Use your spreadsheet or calculator to calculate the wavelength calibration coefficients. In your 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**
6. 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 you execute the regression, an output similar to the one shown below is obtained.

Regression Statistics

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

R Squared

intercept

	Coefficients	Standard Error
Intercept	190.473993	0.369047536
X Variable 1	0.36263983	0.001684745
X Variable 2	-1.174416E-05	8.35279E-07
X Variable 3	-2.523787E-09	2.656608E-10

first coefficient

second coefficient

third coefficient

The numbers of importance are indicated in the above figure.

7. Record the Intercept as well as the First, Second, and Third Coefficients. Also, look at the value for R squared. It should be *very* close to one. If it is not, you have probably assigned one of your wavelengths incorrectly. Keep these values at hand.

Saving the New Calibration Coefficients: USB Mode

Wavelength calibration coefficients unique to each NIRQuest Spectrometer are programmed into an EEPROM memory chip on the NIRQuest Spectrometer.

You can save over old calibration coefficients with new ones and the spectrometer operating software can read these coefficients, *but only if you are using the NIRQuest Spectrometer via the USB port*.

► *Procedure*

To Save Wavelength Calibration Coefficients Using the USB Mode:

1. Ensure that the NIRQuest Spectrometer is connected to the PC and that no other applications are running.
2. Point your browser to http://www.oceanoptics.com/technical/softwaredownloads.asp and scroll down to Microcode. Double-click on **USB EEPROM Programmer**.
3. Save the setup file to your computer.
4. Run the **Setup.exe** file to install the software
5. At the **Welcome** screen, click the **Next** button.
6. At the **Destination Location** screen, accept the default or click the **Browse** button to pick a directory. Then, click the **Next** button.
7. Select a Program Manager Group and click the **Next** button. The Start Installation screen appears. Click the **Next** button.
8. Click the **Finish** button when the Installation Complete screen appears.
9. Reboot the computer when prompted.
10. Navigate to USB EEPROM Programmer and open the software.
11. Click on the NIRQuest Spectrometer device, located in the left pane of the USB Programmer screen.
12. 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.
13. Repeat Step 12 for all of the new values.
14. Click on the **Save All Values** button to save the information, and then **Exit** the USB Programmer software.

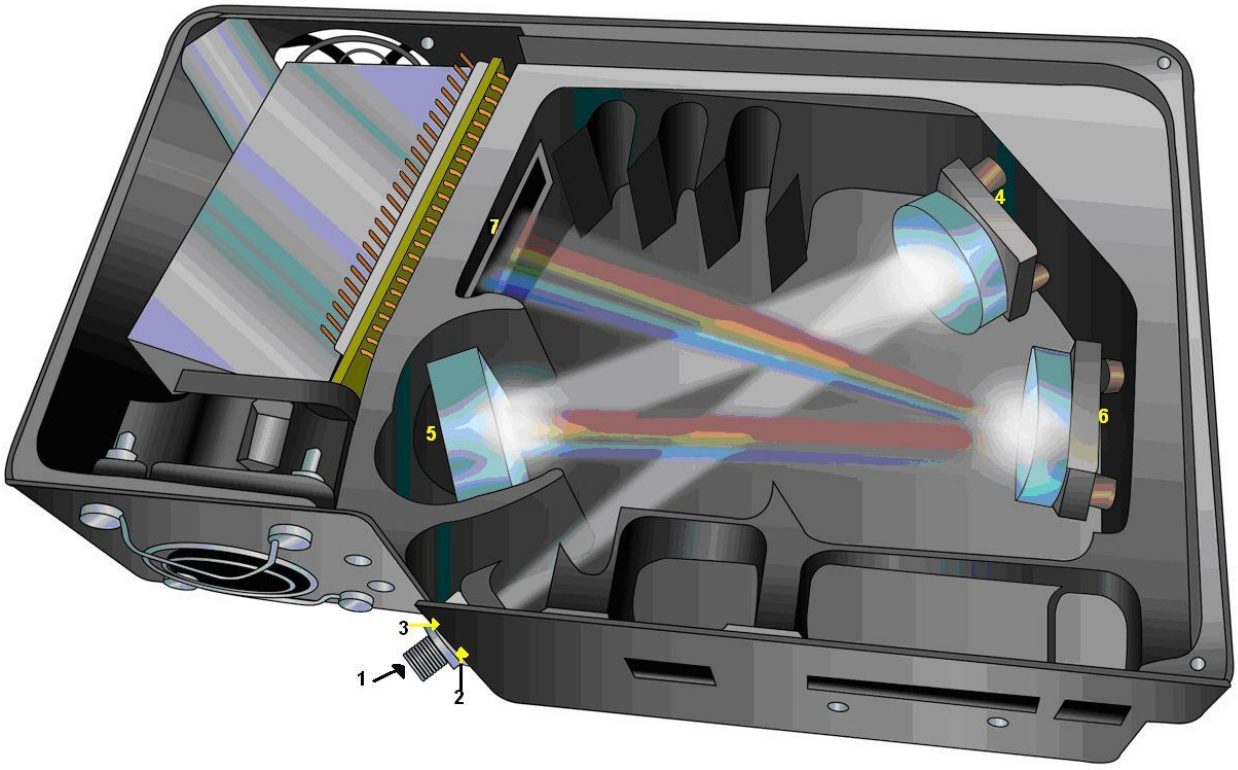
The new wavelength calibration coefficients are now loaded onto the EEPROM memory chip on the NIRQuest Spectrometer.

Appendix B

Specifications

How the Spectrometer Works

Light passes through the NIRQuest Spectrometer through a fixed optical path. The optical bench of the NIRQuest Spectrometer has no moving parts that can wear or break; all the components are fixed in place at the time of manufacture.



NIRQuest Spectrometer with Components

NIRQuest Spectrometer Component Table

The following table describes each component in the NIRQuest Spectrometer. Items marked with an asterisk (*) can be user-specified (consult an Applications Scientist for more information).

1	SMA Connector	Secures the input fiber to the spectrometer. Light from the input fiber enters the optical bench through this connector.
2	Interchangeable Slit	A dark piece of material containing a rectangular aperture, which is mounted directly behind the SMA Connector. The size of the aperture regulates the amount of light that enters the optical bench and controls spectral resolution. You can also use the NIRQuest without a slit. In this configuration, the diameter of the fiber connected to the NIRQuest determines the size of the entrance aperture. The user can change the slit. Ocean Optics also offers a range of FC connector slits in the same wavelengths, with the product code INTFC-XXX. An INTFC-KIT is also available.
3	Filter	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. Only Ocean Optics technicians can change the Filter.
4	Collimating Mirror	Focuses light entering the optical bench towards the Grating of the spectrometer. Light enters the spectrometer, passes through the SMA Connector, Slit, and Filter, and then reflects off the Collimating Mirror onto the Grating.
5	Grating	Diffracts 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. Only Ocean Optics technicians can change the Grating.
6	Focusing Mirror	Receives light reflected from the Grating and focuses the light onto the CCD Detector or L2 Detector Collection Lens (depending on the spectrometer configuration).
7	InGaAs Detector	Each pixel on the detector responds to the wavelength of light that strikes it. Electronics bring the complete spectrum to the software.

NIRQuest512 Specifications

	NIRQuest512-1.7	NIRQuest512-1.9	NIRQuest512-2.2	NIRQuest512-2.5
PHYSICAL				
Dimensions (mm):	182 x 110 x 47			
Weight (kg):	1.18 (w/o power supply)			
DETECTOR				
Detector:	Hamamatsu G9204-512 InGaAs linear array	Hamamatsu G9205-512 InGaAs linear array	Hamamatsu G9206-512 InGaAs linear array	Hamamatsu G9208-512W InGaAs linear array
Detector range:	850-1700 nm	1000-1900 nm	900-2200 nm	900-2550 nm
Useable range[1]:	900-1700 nm	1000-1900 nm	900-2200 nm	900-2500 nm
Pixels:	512			
Pixel size:	25 µm x 500 µm	25 µm x 250 µm		
Saturation charge:	30 pC (~188 Me- electrons)			
Defective pixels:	0 pixels	<20 pixels		
OPTICAL BENCH				
Design:	f/4, symmetrical crossed Czerny-Turner			
Optional Shutter activation time:	11 ms			
Entrance aperture (standard):	25 µm			
Entrance aperture (custom options):	10 µm, 50 µm, 100 µm and 200 µm (or no slit)			
Grating options (standard):	Grating NIR3, 150 l/mm, 900-1700 nm	Grating NIR3, 100 l/mm, 150 l/mm, 900-1700 nm	Grating NIR2, 100 l/mm, 900-2050 nm	Grating NIR1, 75 l/mm, 1075-2500 nm
Grating options (custom)[2]:	NIR10, NIR11, NIR12, NIR13 and NIR14		NIR2, NIR3, NIR10, NIR11, NIR12 and NIR13	

	NIRQuest512-1.7	NIRQuest512-1.9	NIRQuest512-2.2	NIRQuest512-2.5
Longpass filter[3]:	OF1-RG830 longpass NIR filter (optional)	OF1-CGA1000 longpass NIR filter (standard)	OF1-RG830 longpass NIR filter (optional)	
2nd Order filter[3]:	N/A	Standard		
Collimating and focusing mirrors:	Gold-coated for enhanced NIR reflectivity			
Fiber optic connector:	SMA 905 to 0.22 numerical aperture single-strand optical fiber			
SPECTROSCOPIC				
Wavelength range:	900-1700 nm w/Grating NIR3	1100-1900nm w/Grating NIR3	900-2200nm w/Grating NIR2	900-2500nm w/Grating NIR1
Optical resolution (FWHM)[4]:	~3.1 nm w/25 µm slit		~5 nm w/25 µm slit	~6.3 nm w/25 µm slit
Signal-to-noise ratio at full signal[5]:	>15000:1 @ 100 ms integration		10000:1 @ 100 ms integration	
	>13000:1 @ 1000 ms integration			
A/D resolution:	16-bit			
Dark noise:	6 RMS counts @ 100 ms			16 RMS counts@ 10ms
	12 RMS counts @ 1000 ms	12 RMS counts @ 250 ms		24 RMS counts@ 30ms
Dynamic range:	150 x 10^6 (system); 15K:1 for a single acquisition	7.5M (system); 10K:1 for a single acquisition		100K (system); 7.5K:1 for a single acquisition
Integration time[6]:	1 ms – 120 s	1 ms – 1 s		1 ms – 200 ms
Corrected linearity:	>99.8%			>99.6%
ELECTRONICS				
Power consumption	DC input jack +5V, 3 A maximum			
Data transfer speed:	Full scan to memory every 5 ms with USB 2.0 port			
Inputs/ Outputs:	External trigger input + single strobe output			

	NIRQuest512-1.7	NIRQuest512-1.9	NIRQuest512-2.2	NIRQuest512-2.5
Breakout box compatibility:	Yes			
Trigger modes:	2 modes (Normal/Free Run + External Hardware Edge Trigger)			
Strobe functions:	Yes			
Gated delay:	Yes, with external hardware trigger delay			
Connector:	30-pin connector			
TEMPERATURE & THERMOELECTRIC COOLING				
Temperature limits (environmental):	10-35 ºC (0-90% non-condensing)			
TEC range:	20 -- 35ºC below ambient	30 -- 50ºC below ambient		
TEC stability:	+/-0.5 ºC of set temperature in <1 minute; typical long-term stability +/-0.1 ºC			
COMPUTER				
Computer interfaces:	USB 2.0 @ 480 Mbps; RS-232 (2-wire) @ 115.2 K baud (custom configuration)			
Peripheral interfaces:	I2C inter-integrated circuit			

[1] "Useable range" is defined in the context of the NIRQuest model's detector response and its typical grating response. For example, the 512-element detector has response at 850 nm, but grating response begins at 900 nm. The G9206 256-element detector response is sensitive to TEC temperature, and has response only to 2050 nm when the TEC is set to -20 ºC. The G9208 256-element and 512-element detector has response to 2550 nm, but the grating efficiency drops off at 2500 nm.

[2] See *NIRQuest Gratings* for more information.

[3] Other filter options are available for order-sorting in the NIRQuest 512-2.5. NIRQuest 512-2.5 ship with a 2nd-order filter. See an Applications Scientist for details.

[4] Optical resolution (FWHM) depends on grating and slit selection.

[5] SNR will decrease at longer integration times.

[6] Maximum integration times are defined as the longest amount of time one can integrate the spectrometer before the dark level rises to half of full scale.

NIRQuest256 Spectrometer Specifications

	NIRQuest256-2.1	NIRQuest256-2.5
PHYSICAL		
Dimensions (mm):	182 x 110 x 47	
Weight (kg):	1.18 (w/o power supply)	
DETECTOR		
Detector:	Hamamatsu G9206-256 InGaAs linear array	Hamamatsu G9208-256 InGaAs linear array
Detector range:	900-2100 nm	900-2550 nm
Useable range[1]:	900-2050 nm	900-2500 nm
Pixels:	256	
Pixel size:	50 µm x 250 µm	
Saturation charge:	30 pC (~188 Me- electrons)	
Defective pixels:	<12 pixels	
OPTICAL BENCH		
Design:	f/4, symmetrical crossed Czerny-Turner	
Optional Shutter activation time:	11 ms	
Entrance aperture (standard):	25 µm	
Entrance aperture (custom options):	10 µm, 50 µm, 100 µm and 200 µm (or no slit)	
Grating options (standard):	Grating NIR2, 100 l/mm, 900-2050 nm	Grating NIR1, 75 l/mm, 1075-2500 nm
Grating options (custom)[2]:	NIR2, NIR3, NIR10, NIR11, NIR12 and NIR13	
Longpass filter[3]:	OF1-RG830 longpass NIR filter (optional)	
2nd Order filter[3]:	Standard	
Collimating and focusing mirrors:	Gold-coated for enhanced NIR reflectivity	

	NIRQuest256-2.1	NIRQuest256-2.5
Fiber optic connector:	SMA 905 to 0.22 numerical aperture single-strand optical fiber	
SPECTROSCOPIC		
Wavelength range:	900-2050 nm w/Grating NIR2	900-2500 nm w/Grating NIR1
Optical resolution (FWHM)[4]:	~7.6 nm w/25 µm slit	~ 9.5 nm w/25 µm slit
Signal-to-noise ratio at full signal[5]:	10000:1 @ 100 ms integration	7500:1 @ 10 ms integration
A/D resolution:	16-bit	
Dark noise:	6 RMS counts @ 100 ms	8 RMS counts @ 10 ms
	12 RMS counts @ 250 ms	12 counts RMS @ 30 ms
Dynamic range:	15M (system); 10K:1 for a single acquisition	500K (system); 7.5K:1 for a single acquisition
Integration time[6]:	1 ms – 2 s	1 ms – 400 ms
Corrected linearity:	>99.8%	>99.6%
Estimated Peak Noise Equivalent Power (NEP) (default configuration)	5 pW	25 pW
ELECTRONICS		
Power consumption	DC input jack +5V, 3 A maximum	
Data transfer speed:	Full scan to memory every 5 ms with USB 2.0 port	
Inputs/ Outputs:	External trigger input + single strobe output	
Breakout box compatibility:	Yes	
Trigger modes:	2 modes (Normal/Free Run + External Hardware Edge Trigger)	
Strobe functions:	Yes	
Gated delay:	Yes, with external hardware trigger delay	
Connector:	30-pin connector	

	NIRQuest256-2.1	NIRQuest256-2.5
TEMPERATURE & THERMOELECTRIC COOLING		
Temperature limits (environmental):	10-35 ºC (0-90% non-condensing)	
TEC range:	30 -- 50ºC below ambient	
TEC stability:	+/-0.5 ºC of set temperature in <1 minute; typical long-term stability +/-0.1 ºC	
COMPUTER		
Computer interfaces:	USB 2.0 @ 480 Mbps; RS-232 (2-wire) @ 115.2 K baud (custom configuration)	
Peripheral interfaces:	I2C inter-integrated circuit	

[1] "Useable range" is defined in the context of the NIRQuest model's detector response and its typical grating response. For example, the 512-element detector has response at 850 nm, but grating response begins at 900 nm. The G9206 256-element detector response is sensitive to TEC temperature, and has response only to 2050 nm when the TEC is set to -20 ºC. The G9208 256-element and 512-element detector has response to 2550 nm, but the grating efficiency drops off at 2500 nm.

[2] See *NIRQuest Gratings* for more information.

[3] Other filter options are available for order-sorting in the NIRQuest256-2.1, NIRQuest256-2.5 and NIRQuest 512-2.5. NIRQuest256-2.5 and NIRQuest 512-2.5 ship with a 2nd-order filter. See an Applications Scientist for details.

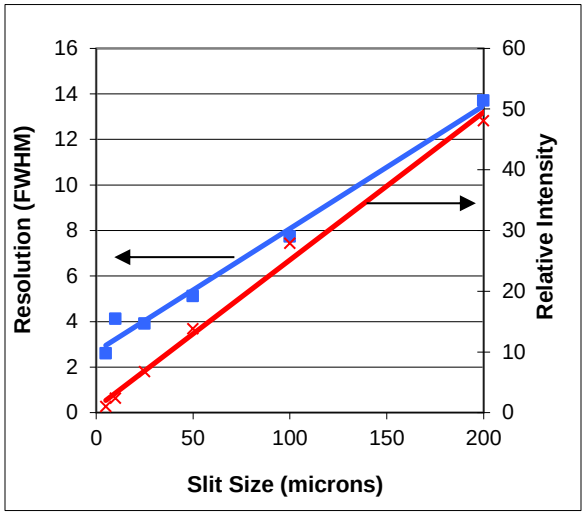
[4] Optical resolution (FWHM) depends on grating and slit selection.

[5] SNR will decrease at longer integration times.

[6] Maximum integration times are defined as the longest amount of time one can integrate the spectrometer before the dark level rises to half of full scale.

NIRQuest Spectrometer – Slit Size vs. Resolution and Throughput

The following chart illustrates the effect that varying slit sizes have on NIRQuest512 Spectrometer resolution and throughput:



NIRQuest Gratings

The following tables show the NIRQuest gratings available for preconfigured (standard) setups and for all options. Additional grating options, adjustments to starting and ending wavelengths and similar customization may be available. Please contact an Applications Scientist for details.

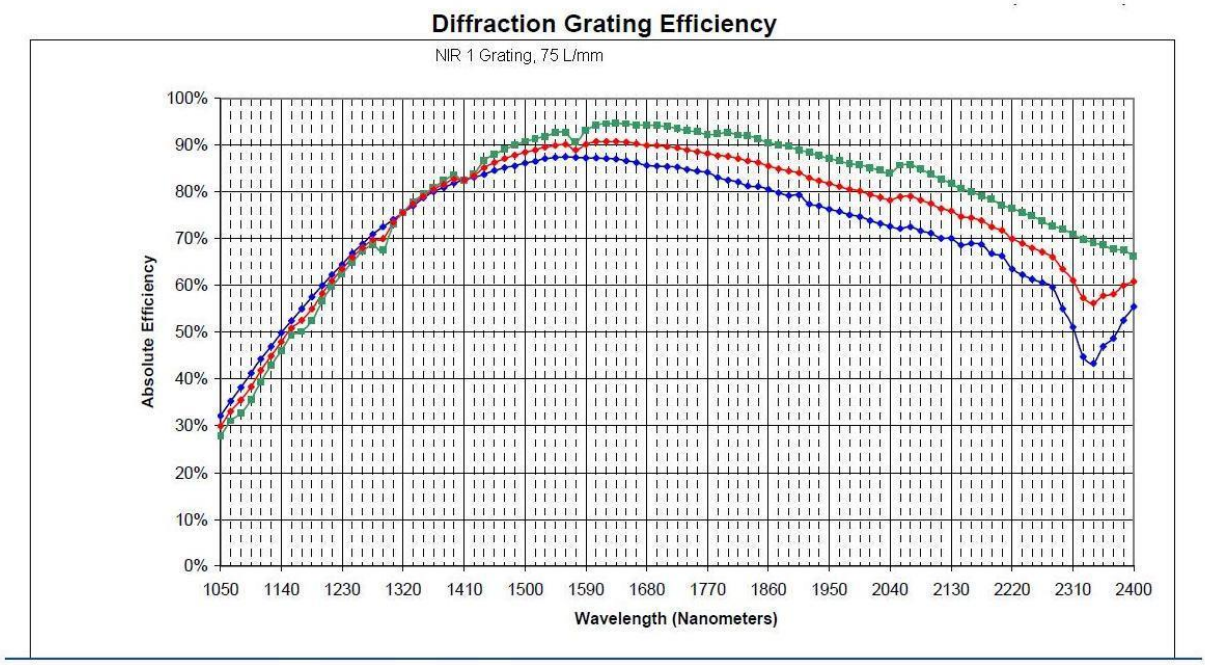
Spectrometer	Standard Grating	Groove Density (lines/mm)	Spectral Range	Blaze Wavelength	Best Efficiency (>30%)
NIRQuest512-1.7	NIR3	150	~800 nm	1100 nm	900-1700 nm
NIRQuest512-1.9	NIR3	150	~800 nm	1100 nm	1100-1900 nm
NIRQuest512-2.2	NIR2	100	1150 nm	1600 nm	900-2200 nm
NIRQuest512-2.5	NIR1	75	1425 nm	1700 nm	1075-2500 nm
NIRQuest256-2.1	NIR2	100	1150 nm	1600 nm	900-2050 nm
NIRQuest256-2.5	NIR1	75	1425 nm	1700 nm	1075-2500 nm

NIRQuest Gratings – All Options

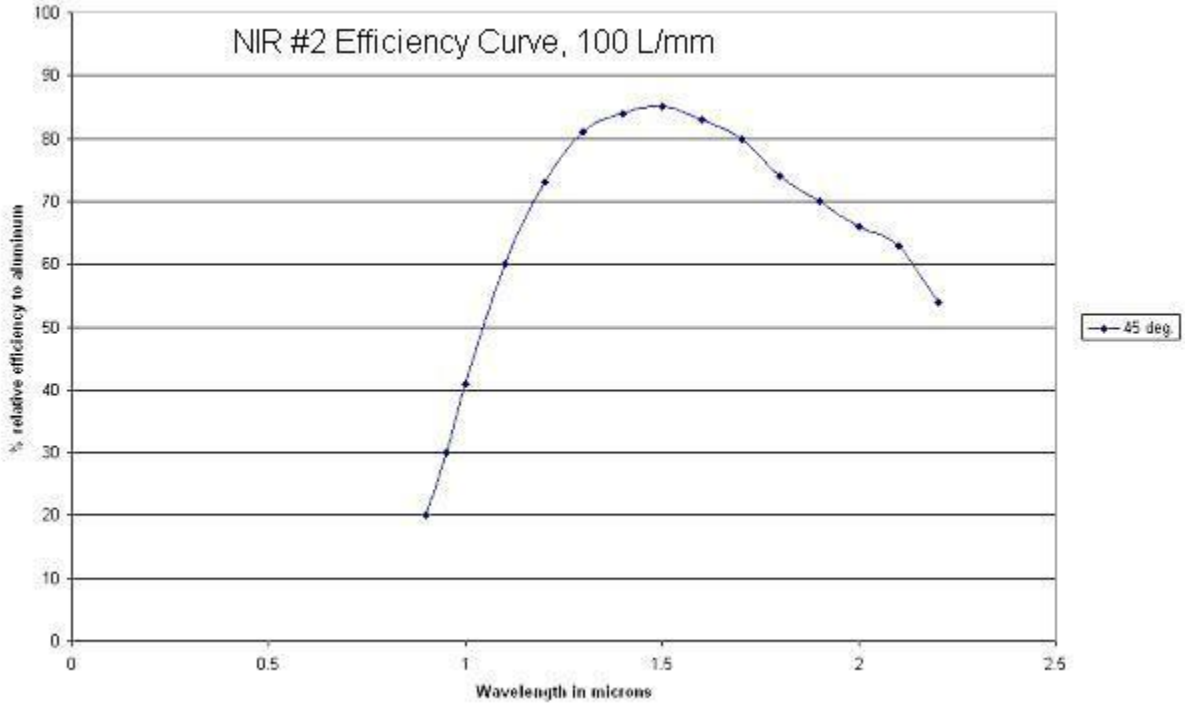
Grating	Intended Use	Groove Density (lines/mm)	Spectral Range*	Blaze Wavelength	Best Efficiency (>30%)
NIR1	NIRQuest512-2.5 NIRQuest256-2.5	75	1600 nm	1700 nm	1075-2500 nm
NIR2	NIRQuest 512-2.2 NIRQuest512-2.5 NIRQuest256-2.1 NIRQuest256-2.5	100	1200 nm	1600 nm	900-2050 nm
NIR3	NIRQuest512-1.7 NIRQuest512-1.9 NIRQuest512-2.2 NIRQuest 512-2.5 NIRQuest256-2.1 NIRQuest256-2.5	150	~800 nm	1100 nm	900-1700 nm
NIR10	NIRQuest512-1.7 NIRQuest512-2.2 NIRQuest512-2.5 NIRQuest256-2.1 NIRQuest256-2.5	300	350-380 nm	1200 nm	750-2200 nm
NIR11	NIRQuest512-1.7 NIRQuest512-2.2 NIRQuest512-2.5 NIRQuest256-2.1 NIRQuest256-2.5	400	240-290 nm	1600 nm	980-2500 nm
NIR12	NIRQuest512-1.7 NIRQuest512-2.2 NIRQuest512-2.5 NIRQuest256-2.1 NIRQuest256-2.5	500	160-220 nm	1370 nm	900-2500 nm
NIR13	NIRQuest512-1.7 NIRQuest512-2.2 NIRQuest512-2.5 NIRQuest256-2.1 NIRQuest256-2.5	600	100-180 nm	1200 nm	800-2500 nm
NIR14	NIRQuest512	1000	50-90 nm	1310 nm	900-1700 nm
* The spectral range is a function of the starting wavelength; the longer (i.e., the farther out in the NIR) the starting wavelength, the smaller the spectral range possible.					

Grating Efficiency Curves

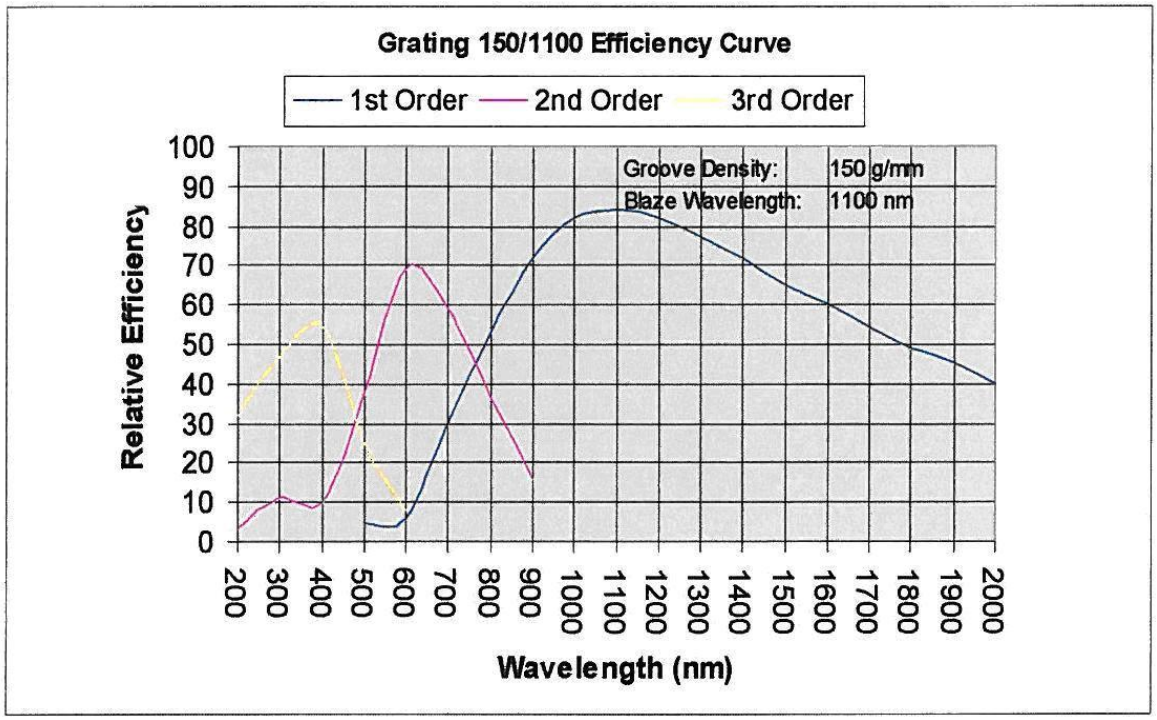
The following graphs show grating efficiency only. System sensitivity is due to several factors, including detector response and grating efficiency.



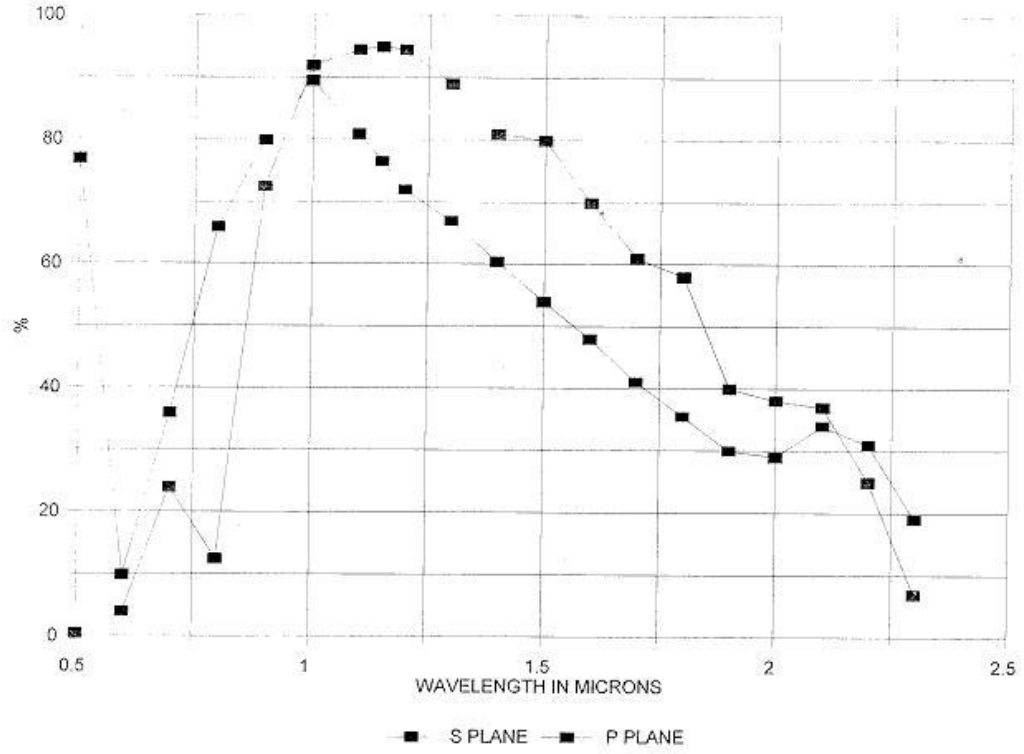
Grating NIR1, 1075 – 2500 nm, 75 l/mm, Blazed at 1700 nm



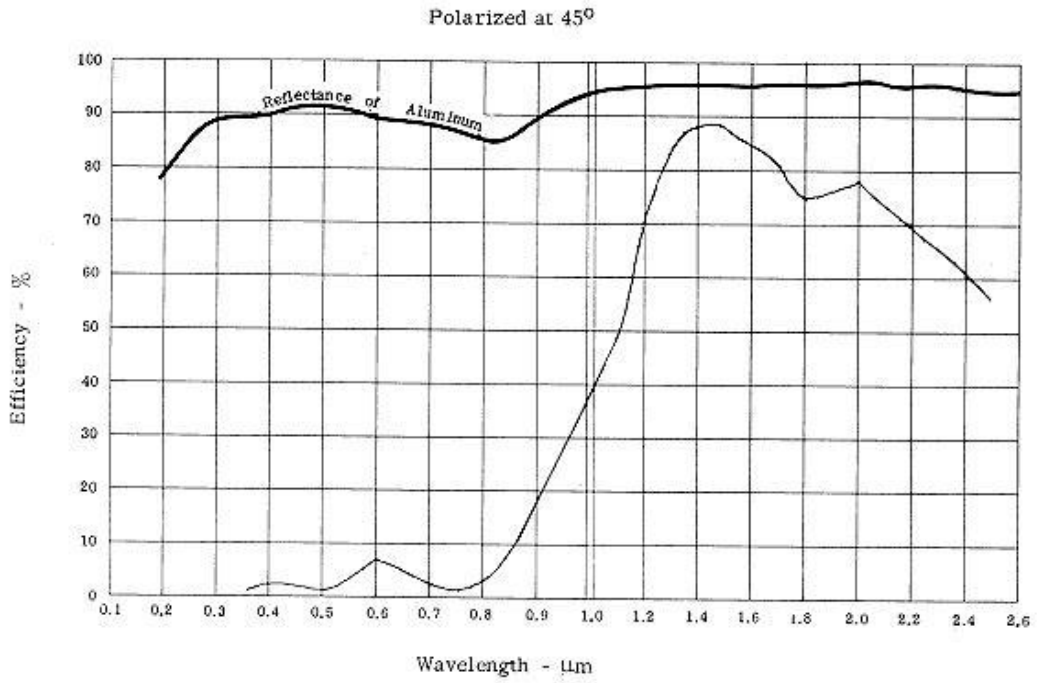
Grating NIR2, 900 – 2050 nm, 100 l/mm, Blazed at 1600 nm



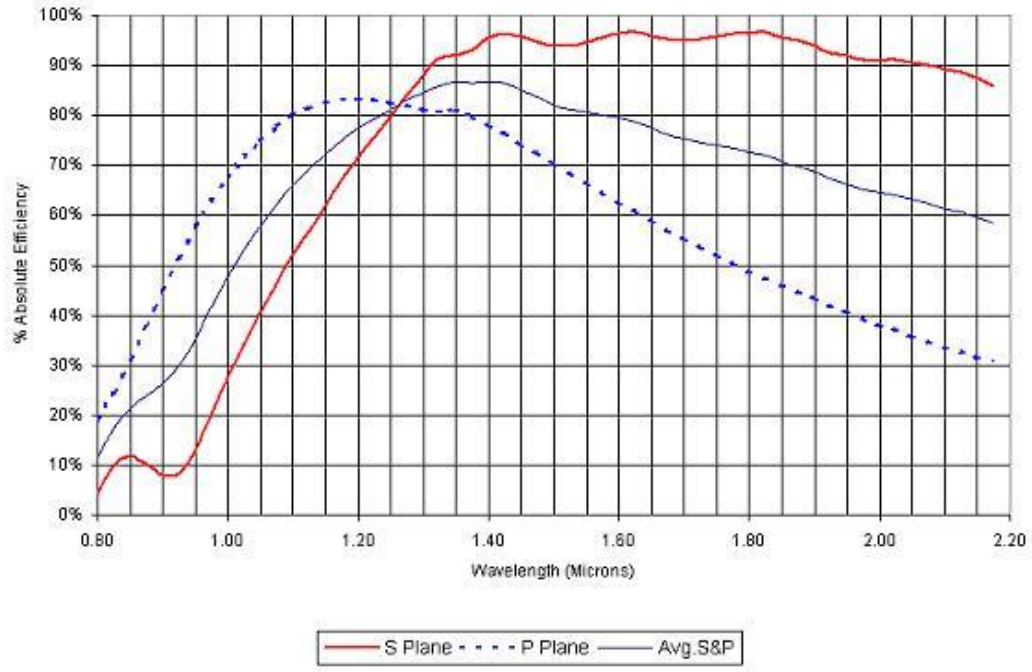
Grating NIR3, 900 – 1700 nm, 150 l/mm, Blazed at 1100 nm



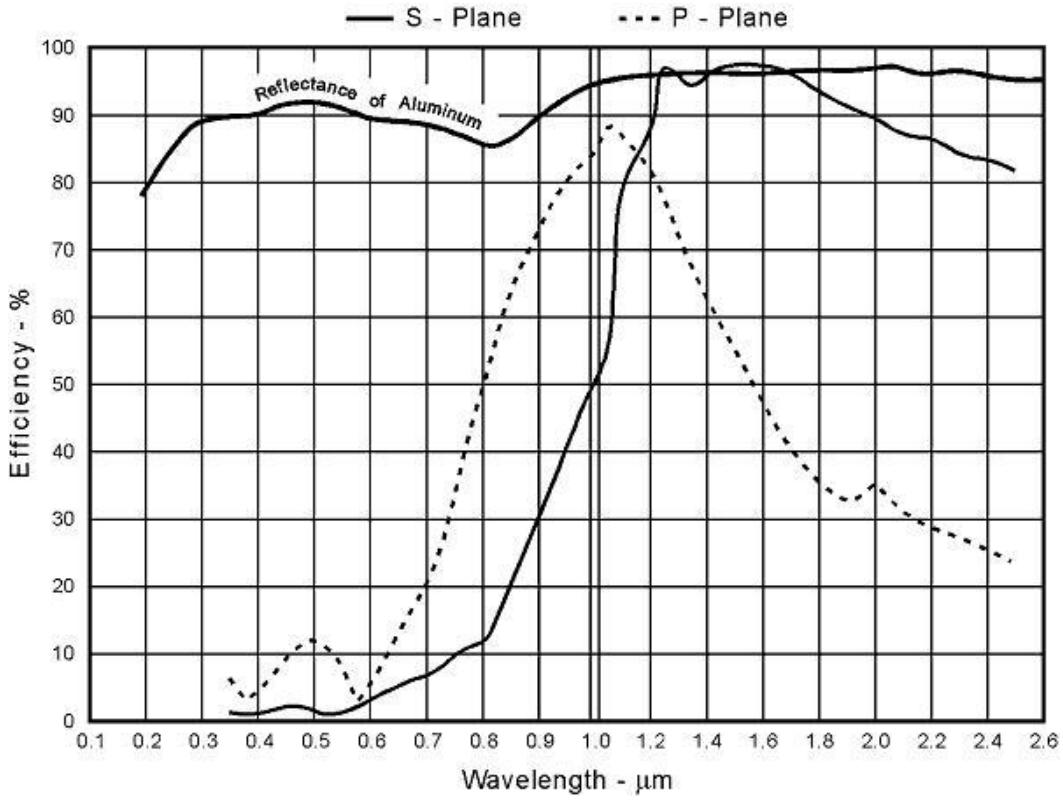
Grating NIR10, 750 – 2200 nm, 300 l/mm, Blazed at 1200 nm



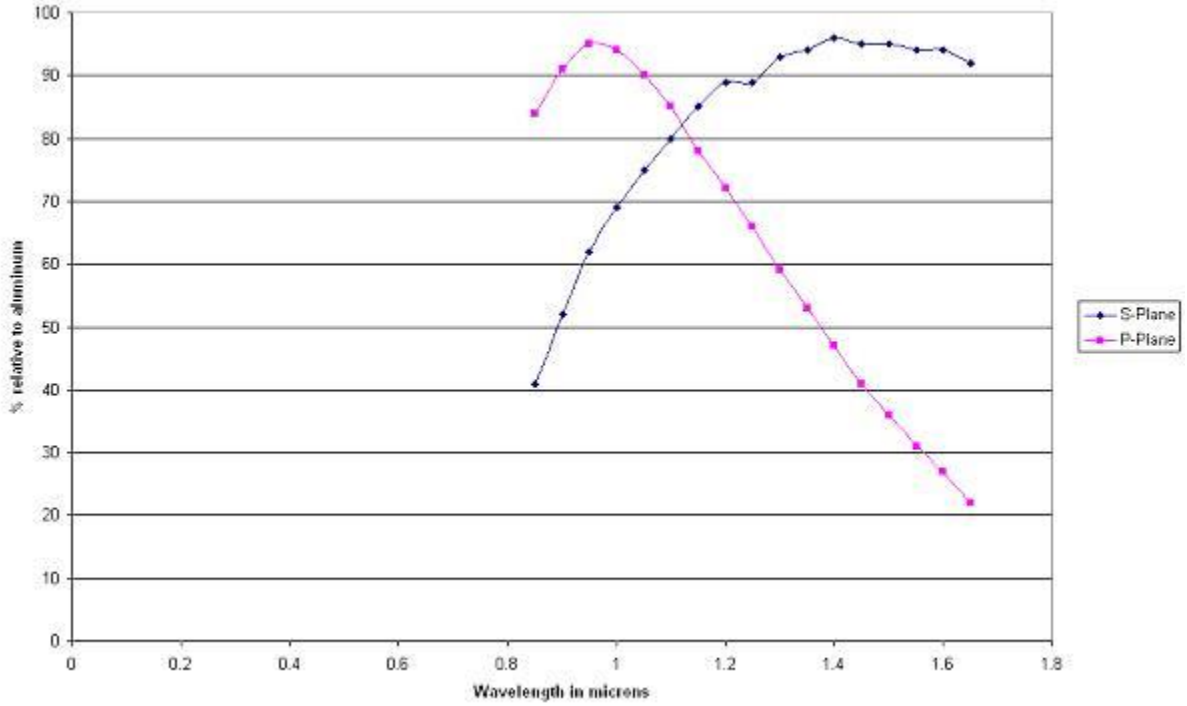
Grating NIR11, 980 – 2500 nm, 400 l/mm, Blazed at 1600 nm



Grating NIR12, 900 – 2500 nm, 500 l/mm, Blazed at 1370 nm



Grating NIR13, 800 – 2500 nm, 600 l/mm, Blazed at 1200 nm



Grating NIR14, 900 – 1700 nm, 1000 l/mm, Blazed at 1310 nm

NIRQuest Optical Resolution for Standard Setups

The following table lists the optical resolution (FWHM) by slit width for standard (preconfigured) setups. Optical resolution will vary by grating range and slit size.

Optical Resolution by Slit Width

Slit	NIRQuest512[1]	NIRQuest512-2.2[2]	NIRQuest512-2.5[3]	NIRQuest256-2.1[2]	NIRQuest256-2.5[3]
SLIT-10	~2.0 nm	~3.0 nm	~4.1 nm	~6.7 nm	~8.3 nm
SLIT-25	~3.1 nm	4.7 nm	~6.3 nm	~7.6 nm	~9.5 nm
SLIT-50	~3.6 nm	~5.4 nm	~7.2 nm	~8.9 nm	~11.1 nm
SLIT-100	~6.6 nm	~9.8 nm	~13.1 nm	~11.2 nm	~13.9 nm
SLIT-200	~12.3 nm	~18.5 nm	~25 nm	~17.9 nm	~22.2 nm

[1] Grating NIR3 used (900-1700 nm)
[2] Grating NIR2 used (900-2050 nm)
[3] Grating NIR1 used (900-2500 nm)

30-Pin Accessory Connector Pinout

The NIRQuest features a 30-pin Accessory Connector, located on the side of the unit as shown:

Location of NIRQuest 30-Pin Accessory Connector

30-Pin Accessory Connector Pinout Diagram

When facing the 30-pin Accessory Connector on the front of the vertical wall of the NIRQuest, pin numbering is as follows:

USB Port

2	4	6	8	10	12	14	16	18	20	22	24	26	28	30
1	3	5	7	9	11	13	15	17	19	21	23	25	27	29

30-Pin Accessory Connector Pinout Diagram

30-Pin Accessory Connector – Pin Definitions and Descriptions

The following table contains information regarding the function of each pin in the NIRQuest's 30-Pin Accessory Connector:

Pin #	Function	Input/Output	Description
1	RS232 Rx	Input	RS232 receive signal –RS-232 functionality is not implemented in software.
2	RS232 Tx	Output	RS232 transmit signal – RS-232 functionality is not implemented in software.
3	GPIO (2)	Input/Output	GPIO

Pin #	Function	Input/Output	Description
4	GPIO (1)	Input/Output	GPIO. Controls the optional shutter.
5	Ground	Input/Output	Ground
6	I^2C SCL	Input/Output	I^2C clock signal for communication to other I^2C peripherals
7	GPIO (0)	Input/Output	GPIO
8	I^2C SDA	Input/Output	I^2C data signal for communication to other I^2C peripherals
9	N/A	N/A	Reserved
10	Ext. Trigger In	Input	TTL input trigger signal
11	GPIO (3)	Input/Output	GPIO
12	V_{CC} or $5V_{IN}$	Input or Output	Input power pin for NIRQuest – When operating via USB, this pin can power other peripherals – Ensure that peripherals comply with USB specifications (no TEC power)
13	SPI Data Out	Output	Reserved
14	V_{CC} or $5V_{IN}$	Input or Output	Input power pin for NIRQuest – When operating via USB, this pin can power other peripherals – Ensure that peripherals comply with USB specifications (no TEC power)
15	SPI Data In	Input	Reserved
16	GPIO (4)	Input /Output	GPIO
17	Single Strobe	Output	TTL output pulse used as a strobe signal – Has a programmable delay relative to the beginning of the spectrometer integration period
18	GPIO (5)	Input/Output	GPIO
19	SPI Clock	Output	Reserved
20	Continuous Strobe	Output	TTL output signal used to pulse a strobe – Divided down from the master clock signal
21	SPI Chip Select	Output	Reserved
22	GPIO (6)	Input/Output	GPIO
23	N/A	N/A	Reserved

Pin #	Function	Input/Output	Description
24	N/A	N/A	Reserved
25	Lamp Enable	Output	TTL signal driven Active HIGH when the Lamp Enable command is sent to the spectrometer
26	GPIO (7)	Input/Output	GPIO
27	Ground	Input/Output	Ground
28	GPIO (8)	Input/Output	GPIO
29	Ground	Input/Output	Ground
30	GPIO (9)	Input/Output	GPIO

30-Pin J2 Accessory Connector - Part Numbers

The part numbers for the 30-pin accessory connector on the NIRQuest Spectrometer are as follows:

- The connector is Pak50™ model from 3M Corp. Headed Connector – Part Number **P50–030P1–RR1–TG**.
- The mating connector is Part Number **P50–030S–TGF**.
- Mating the two components requires two 1.27 mm (50 mil) flat ribbon cables (3M 3365 Series is recommended).

NIRQuest 15-Pin Accessory Cable Pinout

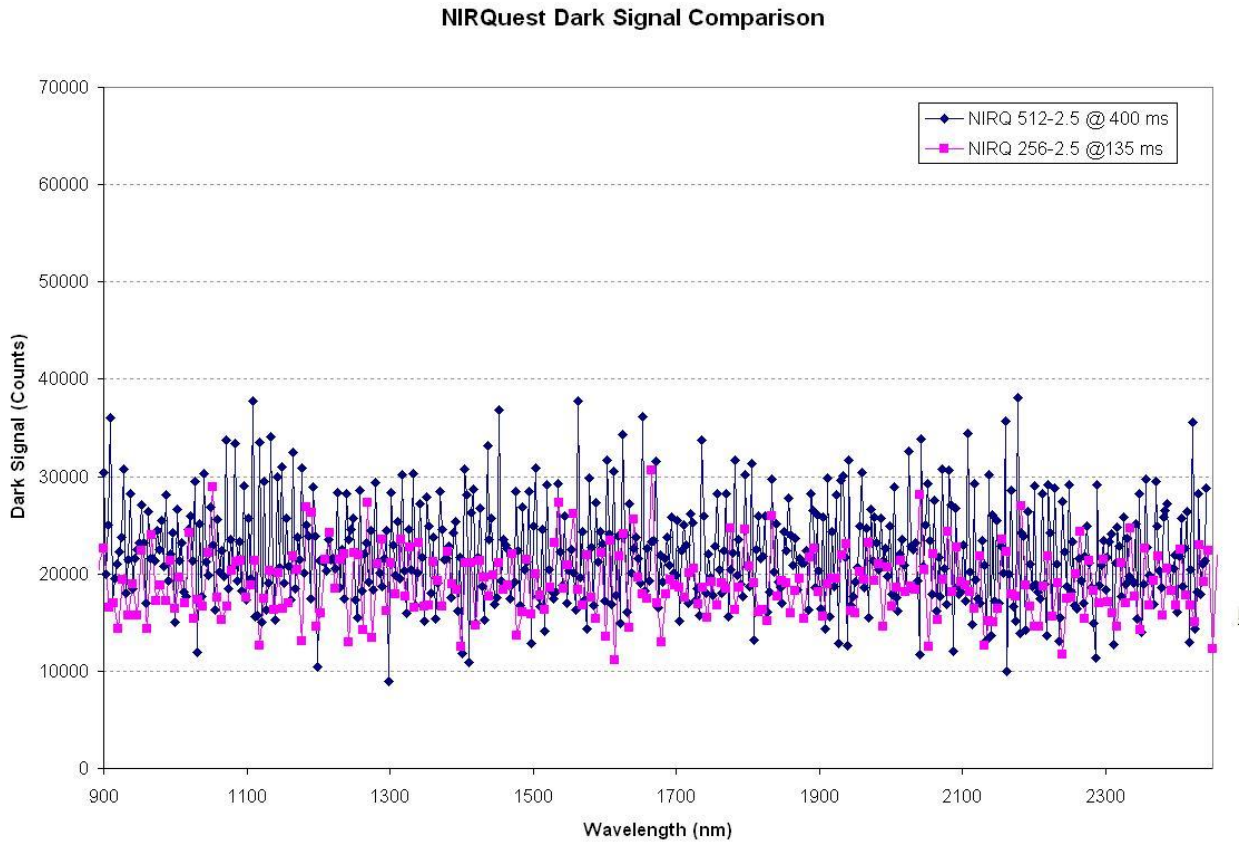
Pin #	Description	Pin #	Description
1	Single_strobe	9	GPIO-9
2	ContStrobe	10	GND_SIGNAL
3	V5_SW	11	SDA
4	ExtTrigIn	12	SCL
5	ExtTrigIn	13	LampEnable
6	GPIO-8	14	A_IN
7	A_OUT	15	GPIO-7
8	ExtTrigIn		

Appendix C

NIRQuest512-2.5 and NIRQuest256-2.5 Sensitivity

When configuring a system for operation out to 2.5µm it is important that you consider the following details:

- Short Integration Times: For the detector to be sensitive out to 2.5µm, the detector's band gap energy must be small. Unfortunately, this raises the absolute level of the detectors dark signal. Typical dark signals at 400ms (NIRQuest512-2.5) and 135ms (NIRQuest256-2.5) are shown below.
- Fiber Selection: For maximum signal intensity, alternative fiber materials should be used for wavelengths greater than 2.2µm.



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