



thermo scientific

Raman

# iXR Raman Spectrometer

## User Guide

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SCIENTIFIC

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**For Research Use Only. This instrument or accessory is not a medical device and is not intended to be used for the prevention, diagnosis, treatment or cure of disease.**



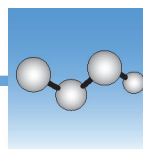
**WARNING** Avoid an explosion or fire hazard. This instrument or accessory is not designed for use in an explosive atmosphere.

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# Using Your iXR Raman Spectrometer

The Thermo Scientific™ iXR Raman spectrometer is the first compact Raman developed specifically for integration and multi-modal analysis with other analytical techniques. Multi-modal analysis with the iXR enhances the understanding of materials by providing detailed molecular level information. With performance comparable to laboratory research grade Raman spectrometers, it is suitable for demanding research, product development and manufacturing needs.

## Conventions Used

This document includes precautions and other important information presented in the following format:



**WARNING** Indicates a hazardous situation which, if not avoided, could result in death or serious injury.

**NOTICE** Follow instructions with this label to avoid damaging the system hardware or losing data.

**Note** Contains helpful supplementary information.

## Safety Precautions



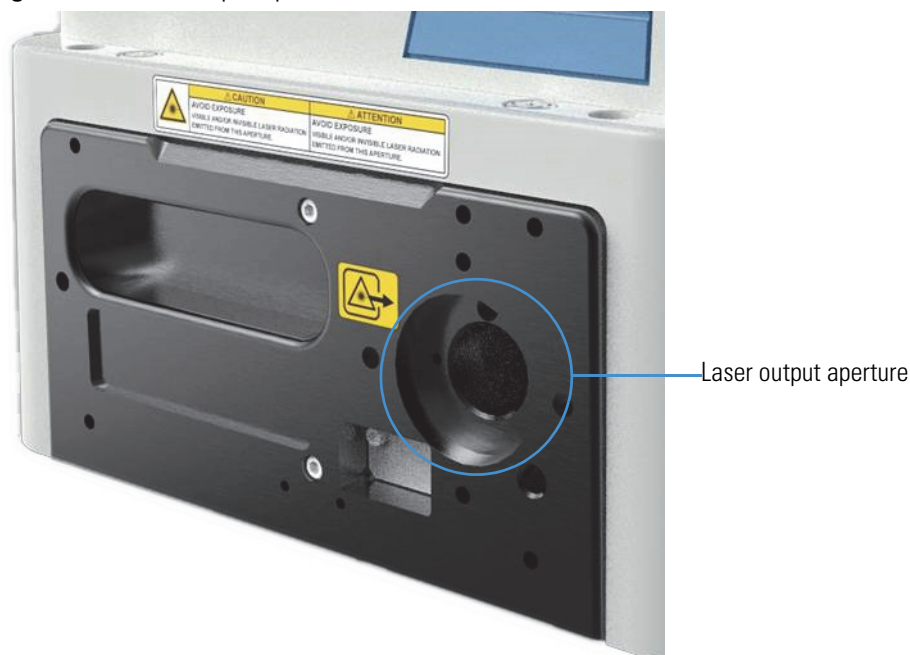
**NOTICE** Be sure that all persons operating this system read the site and safety manual first.



**WARNING** Avoid personal injury. Class 3B instruments should always be operated in a laser safety area.

- All persons using or in the vicinity of a Class 3B instruments should wear appropriate laser safety glasses and should be aware of the potential hazards.
- Use of controls or adjustments or performance of procedures other than those specified in the documentation may result in hazardous radiation exposure.
- The laser energy from the excitation lasers may be visible or invisible.
- Never stare directly into the laser beam or at its bright reflection, even if you are wearing laser safety glasses.

**Figure 1.** Laser output aperture



**NOTICE** Use of equipment and accessories not supplied by us can result in permanent damage to the instrument and may create a safety hazard.

- When operating our Raman instruments, use only accessories and equipment (such as power supplies and lasers) supplied by us.
- Do not attempt to service a laser that is not functioning properly. If a laser is malfunctioning, contact us.

**Note** See the “Manufacturer’s laser information” section in the safety notice that was included with your instrument for information about individual excitation lasers.

## Safety Goggle Specifications



**WARNING** Always wear safety glasses that meet the specifications listed below for your laser(s) whenever there is potential laser emission.

Never stare directly into a laser beam or its reflection, even if you are wearing laser safety glasses. The glasses will protect you for diffuse viewing only.

**785 nm NIR diode laser:** Wear glasses that have an optical density of at least 3 and are rated for wavelengths of 785 nm.

**532 nm green laser:** Wear glasses that have an optical density of at least 3 and are rated for wavelengths of 532 nm.

**633 nm red laser:** Wear glasses that have an optical density of at least 3 and are rated for wavelengths of 633 nm.

**455 nm blue laser:** Wear glasses that have an optical density of at least 3 and are rated for wavelengths of 455 nm.

## Setting up a Laser Safety Area

If you are going to use a Class 3B laser product the instrument must be connected to an external remote interlock system that blocks the laser beam whenever a safety perimeter around the instrument is breached (when an unauthorized person opens the door, for example).

The **maximum permissible exposure (MPE)** is the level of laser radiation that a person may be exposed to, under normal circumstances, without suffering adverse effects. (These levels are based on the assumption that a person is exposed to the laser beam for an infinite length of time.) The **nominal ocular hazard distance (NOHD)** is the distance from the laser output aperture within which the level of laser radiation exceeds the MPE.

### MPE and NOHD values for the system

Laser	MPE (W/m <sup>2</sup> )	NOHD (m)	
		10x objective	no objective
455 nm	10.0	0.30	55.45
532 nm	10.0	0.25	59.92
532 nm (high power)	10.0	0.46	59.92
633 nm (high power)	10.0	0.36	85.92
785 nm	14.8	0.37	72.91
785 nm (high power)	14.8	0.81	22.46



**CAUTION** Avoid personal injury.

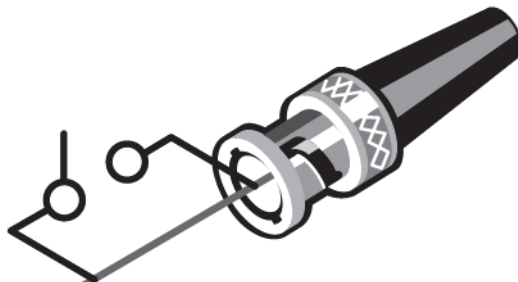
- The connectors and the laser safety circuit must be designed and built by someone who is properly trained.
  - One of our representatives will help you install and test your connector.
  - Please have the connector ready before the system arrives.
- All persons using or in the vicinity of a Class 3B instrument must wear appropriate laser safety glasses and must be aware of the safety precautions.
- The remote interlock system protects all people in the vicinity of the Class 3B laser system.
  - Do not attempt to defeat the interlocks on the system.

**Time needed:** Approximately 5 minutes

**Parts needed:** 2 BNC cables

1. Install a switch across the pins of the connectors on each of the BNC cables.

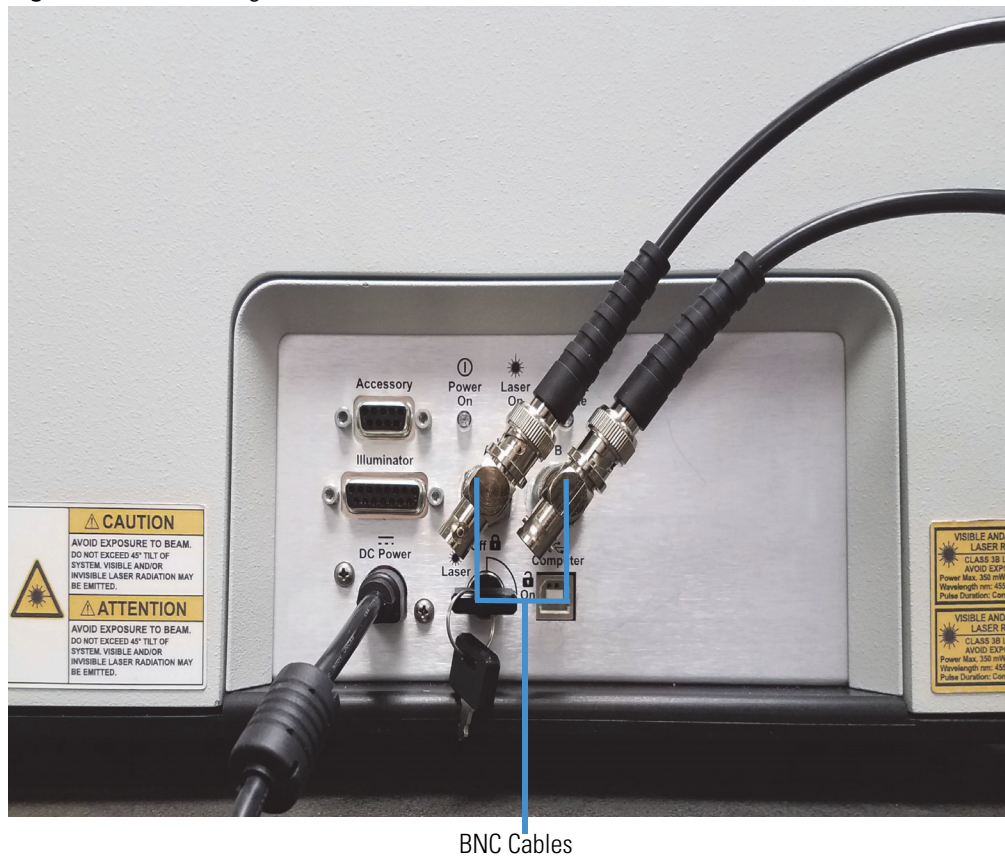
The switch must accommodate +5 VDC at 10 mA while it is closed.



**Note** Opening the switch blocks the laser beam, and closing the switch unblocks the beam.

2. Connect the BNC cables to the BNC connectors on the instrument power panel.

**Figure 2.** Connecting BNC cables



3. Connect the BNC cables to the laser safety circuit you have designed.

## Indicators

**Figure 3.** Instrument indicators



## Operation

The Thermo Scientific™ iXR Raman spectrometer is compatible with several optional accessories and sampling interfaces. This section describes installing and using these components and discusses enabling the laser.

### Attaching the Optional Legs

The optional legs raise the spectrometer off of the work surface and provide extra clearance for sampling interfaces, such as the iXR microscope accessory.

**NOTICE** Avoid damaging the system components. Tipping the system on its side while a laser, filter, or grating is installed could damage the system. Before installing the legs, remove the laser, filter, and grating.

The legs attach to four captive, spring-loaded screws. Installing them requires you to use the screwdriver to push the screws toward to base of the spectrometer so that you can thread the legs onto the screws.

#### Tools Required

- Phillips-head screwdriver, included with the kit
- 4 legs

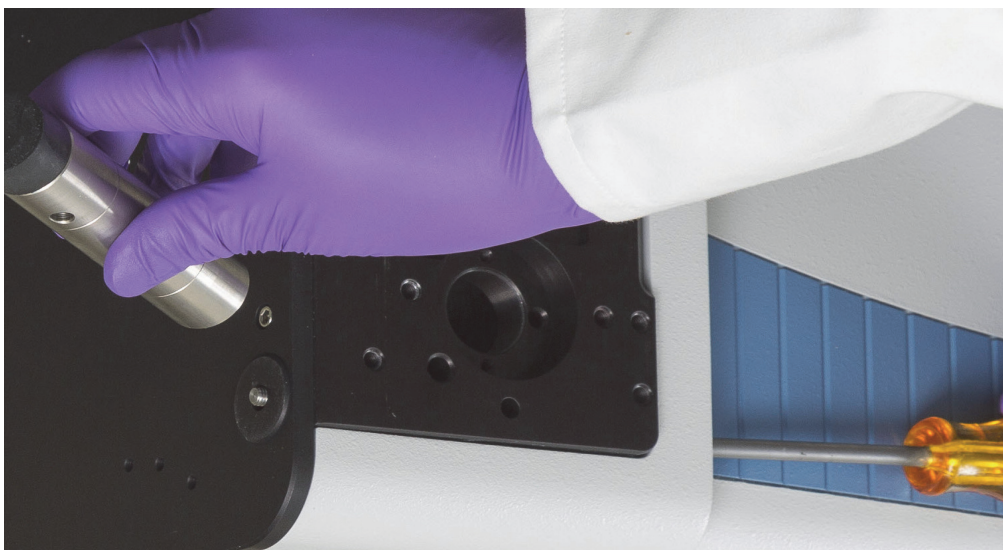
#### ❖ To install the legs

1. Remove the laser, grating, and filter. See [Changing the Laser, Filter and Grating](#) for details.

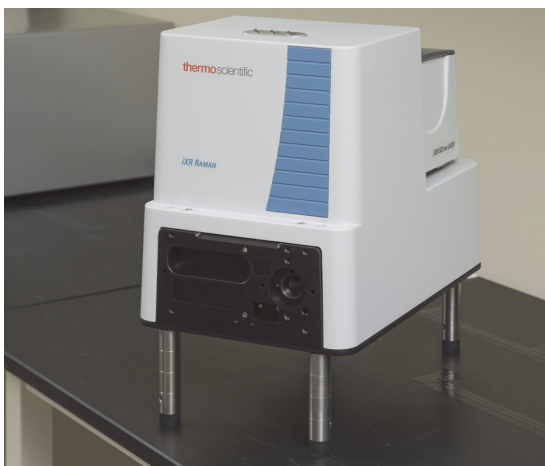


**NOTICE** When tipping the iXR spectrometer, tip it only onto its right side, with the laser compartment toward the work surface. If you tip the spectrometer onto its other side, with the laser compartment away from the work surface, the spectrometer could be damaged.

2. Carefully tip the spectrometer onto its right side, with the laser compartment closer to the work surface.
3. Using the Phillips-head screwdriver, push the captive screws toward to base of the instrument to expose the screw. Thread the leg onto the exposed screw.



4. Using the screwdriver, tighten the screw to fasten the legs securely. It may be easier to use the screwdriver to hold the screw while you turn the legs.
5. Repeat for each of the additional 3 legs.
6. Carefully stand the spectrometer up onto the legs.



## Changing the Laser, Filter and Grating

The primary reason for changing the laser is to avoid a fluorescence response from the sample. When the laser is changed, the filter and grating must also be changed.

The laser, filter, and grating must be removed before shipping the spectrometer or tipping the spectrometer on its side. The filter and grating are held in place by magnets, and they may become detached and may damage the system.

To install the laser, filter, and grating, reverse these procedures.



**WARNING** Avoid shock hazard. Turn off the spectrometer power before you replace or remove the laser, filter, or grating.

### ❖ To remove the laser

1. Pull the black lever away from the laser, rotate the level clockwise 90°. Then, gently pull the laser module away from the spectrometer.

**Figure 4.** Removing the laser



**NOTICE** Handle lasers, filters, and gratings gently. Do not touch any optical surfaces or the interior of a laser, filter, or grating. When a laser, filter, or grating is not in use, store it in the case that it was shipped with.

Store the laser in a safe location.



**❖ To remove the filter**

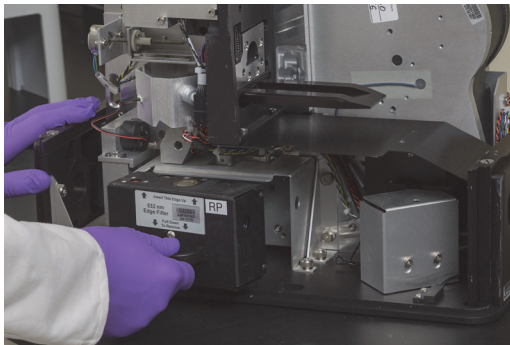
Changing the filter or grating requires you to remove the outer cover from the spectrometer.

1. Use a Phillips-head screwdriver to remove the four captive screws.
2. Lift the cover straight up and away from the instrument.



The filter is held in place by magnets.

3. To remove the filter, gently pull the filter straight out away from the spectrometer.

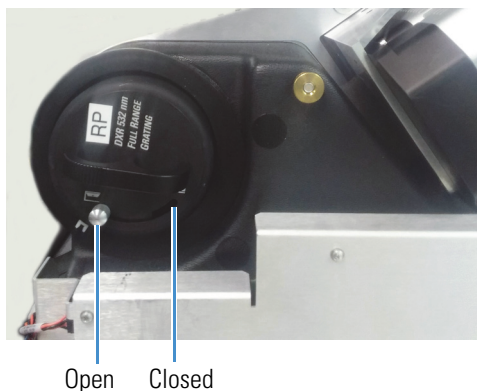


Store the filter in a safe location.

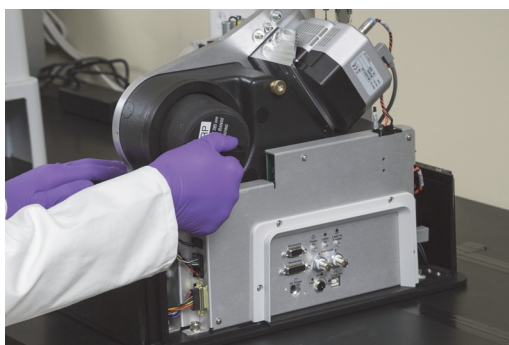
❖ **To change the grating**

The grating is held in place by magnets.

1. With the cover removed, close the protective grating cover by rotating the knob counterclockwise.



2. Gently pull the grating straight out and away from the spectrometer.



3. Use a clean, lint-free cotton cloth to wipe the magnets that secure the grating when installed.

Store the grating in a safe location.

## Enabling the Laser

You must enable the laser before you can turn it on. To enable the laser, rotate the laser key to the locked (vertical) position as shown below. (For more information about turning on the laser, see the software help available through the **Help** menu in OMNIC.)

**Note** You can insert or remove the laser key only when the laser keyswitch is in the unlocked (horizontal) position. When the laser keyswitch is in the unlocked position, the laser is disabled.

**Figure 5.** Laser keyswitch

## Cooling Fans

**NOTICE** To avoid overheating, do not block the free flow of air around the instrument. There should be at least 2 cm (about 1 in) of clearance on each side.

## Connecting and Using a Sampling Interface

Sampling interfaces attach to the spectrometer's laser output aperture. How you connect your sampling interface depends on which interface you have selected.



**WARNING** Avoid permanent eye damage. Visible and/or invisible laser radiation is emitted from this aperture. Wear appropriate laser safety glasses.

Rotate the laser key to the vertical, locked position to disable the laser before installing a sampling interface.

**Figure 6.** Laser output aperture

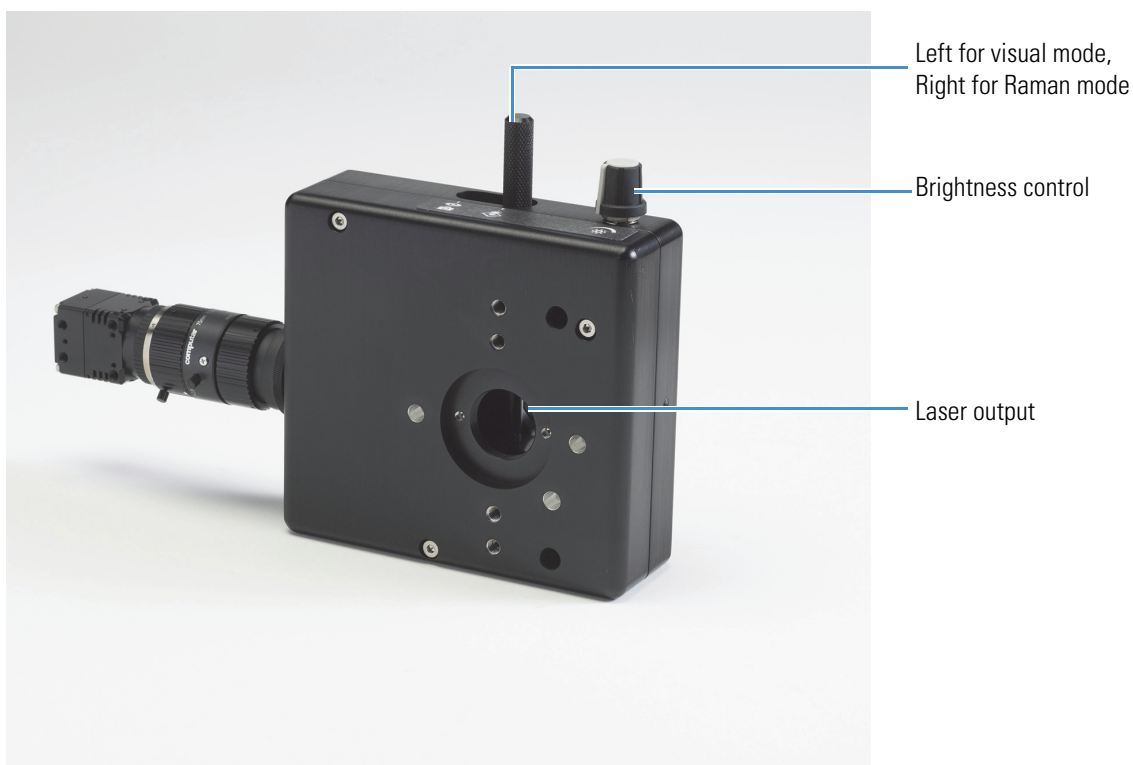


## **iXR Camera Accessory**

The iXR camera accessory can be combined with the microscope accessory, right angle micro accessory, or macro sampling accessory.

When installing the camera with a sampling accessory, the camera mounts to the spectrometer's laser output aperture, and the sampling accessory mounts to the front face of the camera.

Installing the camera requires you to mount the camera to the spectrometer, connect the power cable, and connect the camera to a computer with a USB cable.

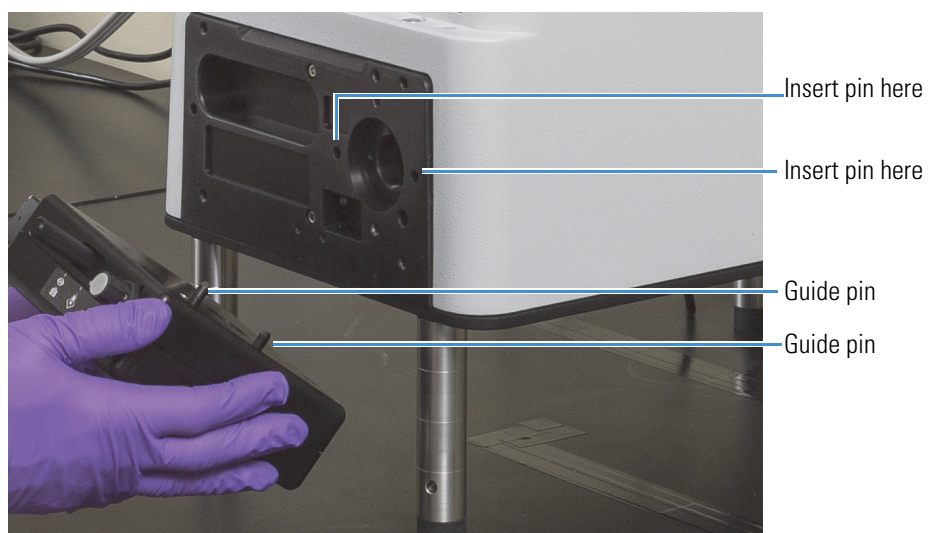


### Required Tools

- 5mm hex driver, supplied

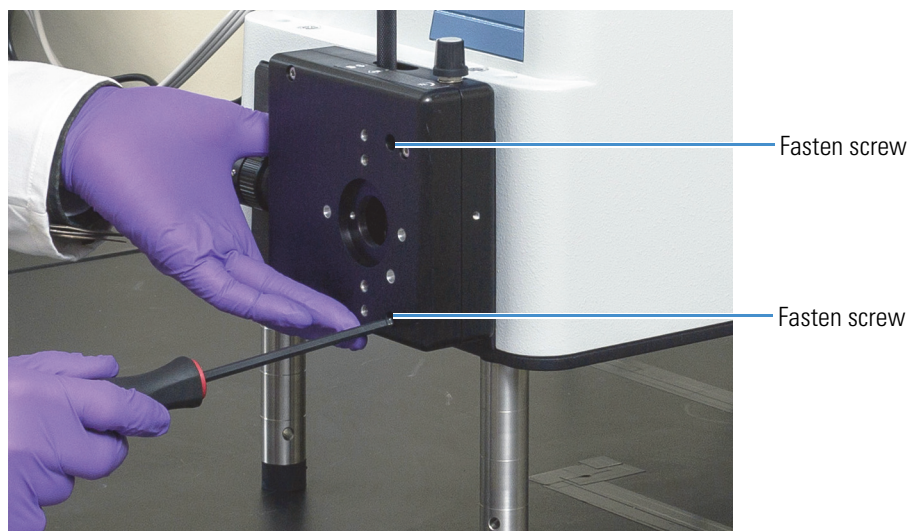
#### ❖ To connect the iXR camera accessory

1. Using the two guide pins on the back of the camera, position the camera over the laser output aperture.

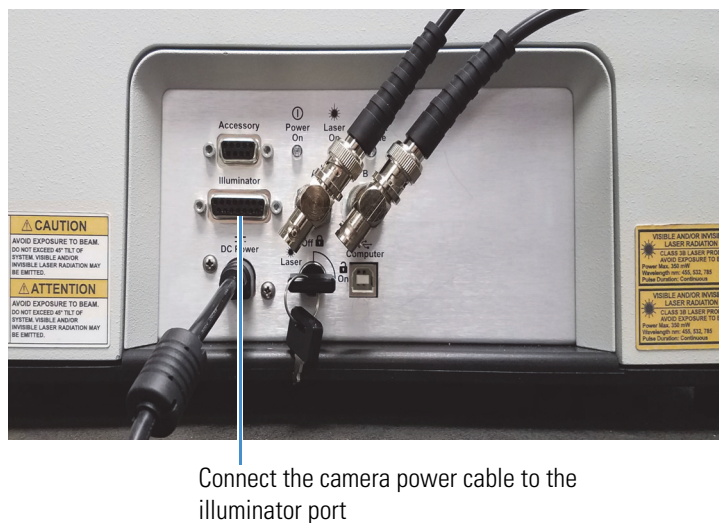




- Using the included 5mm hex driver, fasten the camera to the spectrometer using the two screws captive in the camera body.



- Connect the power cable to the camera and to the illuminator port on the spectrometer.



Connect the camera power cable to the illuminator port

- With the USB cable, connect the camera to a computer.

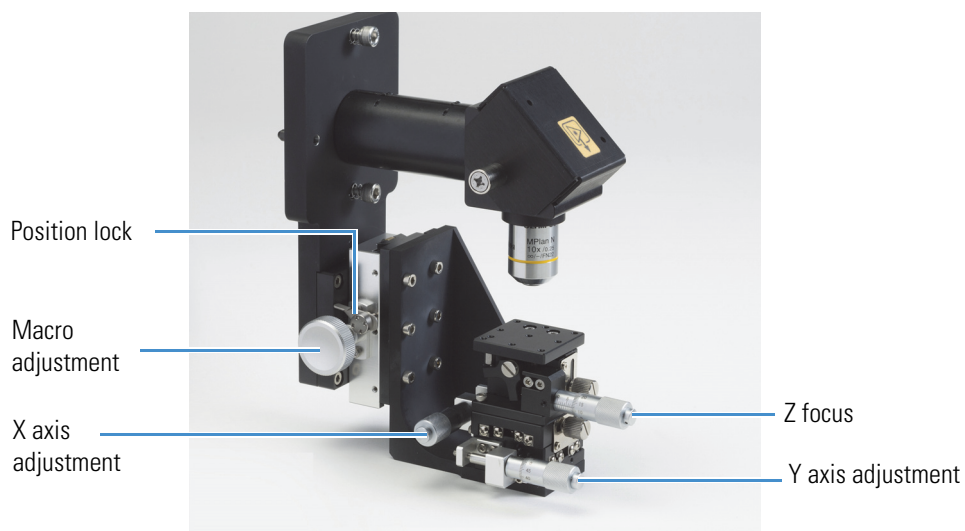
Operate the camera using the StCamSWare software installed with your software package.

### iXR Microscope Accessory

The microscope accessory attaches to the front face of the camera. If desired, the lens tube, right-angle mirror assembly, and objective can be removed from the stage and used as a right angle micro accessory.

To use the iXR Microscope Accessory, first install the legs to raise the instrument off the work surface or bring the instrument to the front edge of the work surface to allow the microscope to hang over the edge.

Mounting the microscope requires you to attach the microscope to the camera, install the objective, and position the mirror assembly over the stage.

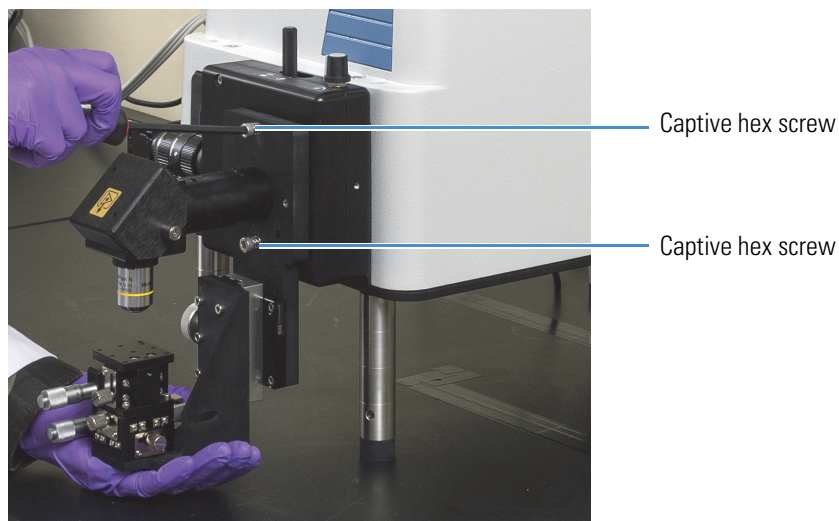


### Required Tools

- 5mm hex driver, supplied
- 5/64" hex driver, supplied

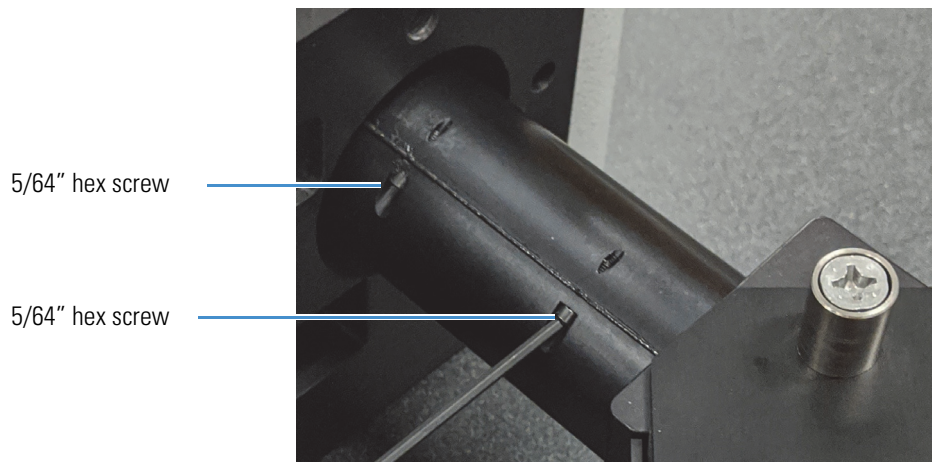
### ❖ To connect the microscope

1. Using the guide pins on the microscope assembly, position the lens tube over the laser output aperture on either the spectrometer or the camera body.
2. Using the supplied 5mm hex driver, fasten the microscope assembly to the face of the camera. The microscope assembly attaches with two captive hex screws, one below and one above the lens tube.



3. Carefully screw the objective into the mirror assembly.

4. Use the 5/64" hex screws on the clamping sleeve of the lens tube to loosen the mirror assembly. With the clamp loosened, rotate the assembly to align the objective over the stage.



If necessary, use the 5/64" hex driver to tilt the turning mirror to align the laser through the lens tube and objective.



### **iXR Right Angle Micro Accessory**

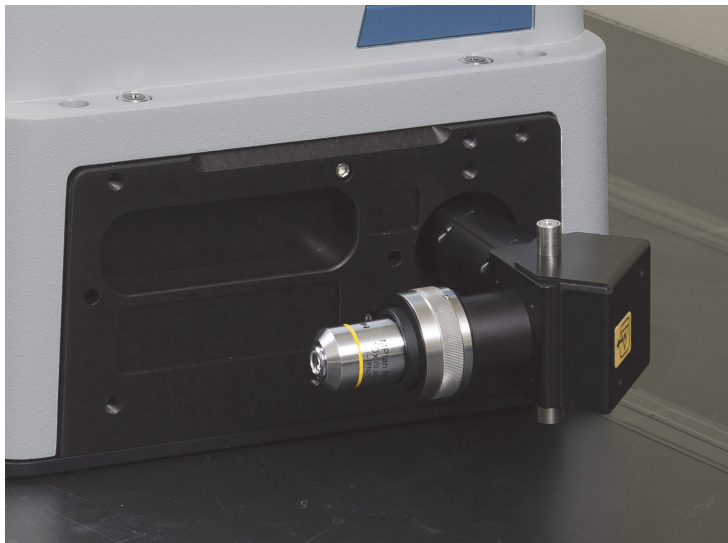
The right angle micro assembly includes the following:

- lens tube with clamping sleeve
- right-angle mirror assembly
- lens tube with focusing ring
- microscope objective



The right-angle micro accessory can be mounted to the front face of the camera accessory or directly to the laser output aperture on the spectrometer.

**Figure 7.** Properly installed iXR right angle accessory



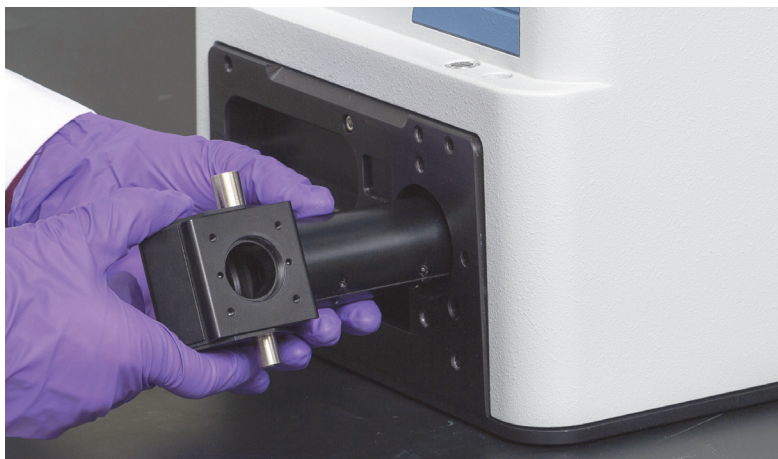
**NOTICE** Avoid damaging the system. Cross threading could damage the instrument or the accessory. To avoid damaging the instrument or the accessory, carefully line up the threads and ensure that the tube is perpendicular to the threading face to avoid cross threading.

❖ **To install the iXR right angle micro accessory**

1. Carefully align the threads and screw the lens tube into the laser output aperture.

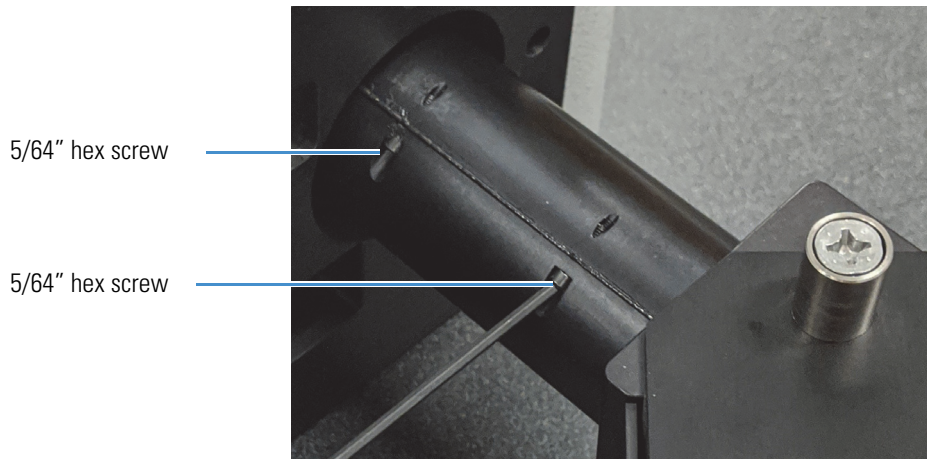
If your spectrometer is not mounted on the legs, you may need to unscrew and remove the lens tube with the focusing ring so that it does not hit the work surface.

**Figure 8.** Attach the lens tube to the laser output aperture



2. Use the 5/64" hex screws to loosen the clamping sleeve and rotate the right-angle mirror assembly into the desired position. Tighten the sleeve to lock the mirror assembly in position.

**Figure 9.** Use the 5/64" hex screws to tighten or loosen the clamping sleeve



3. Carefully align the threads and screw the lens tube with the focusing ring into the mirror assembly.

You can add additional lens tubes to the assembly to extend the mirror farther from the instrument or to move the objective farther from the mirror assembly.

4. Screw the objective into the lens tube.

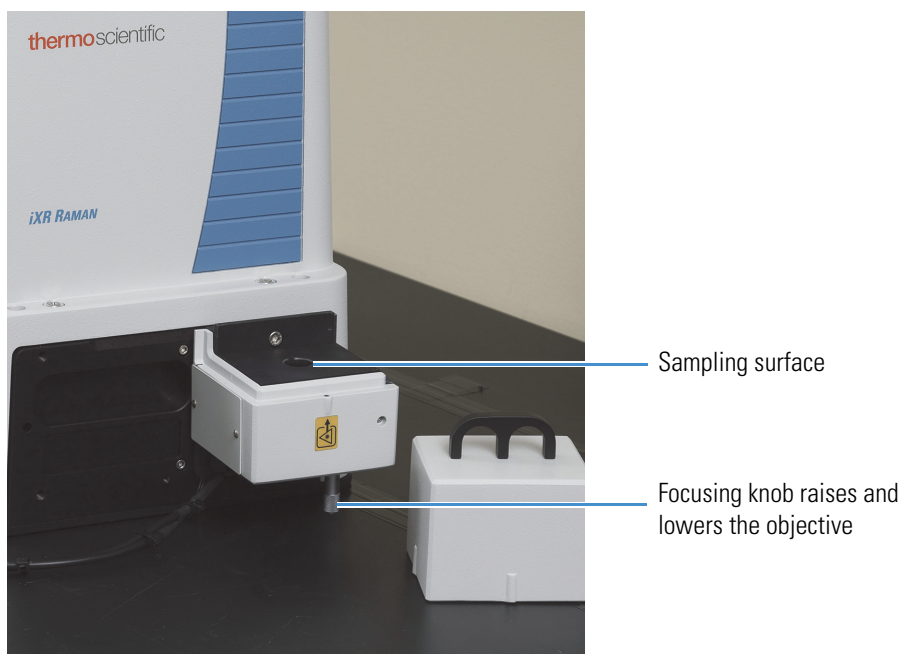


If necessary, use the 5/64" hex driver to tilt the turning mirror to align the laser through the lens tube and objective.



### iXR Macro Sampling Accessory

The macro sampling accessory can be mounted on the camera or directly on the laser output aperture on the spectrometer. The macro sampling accessory includes an interlocked cover that disables the laser when removed.

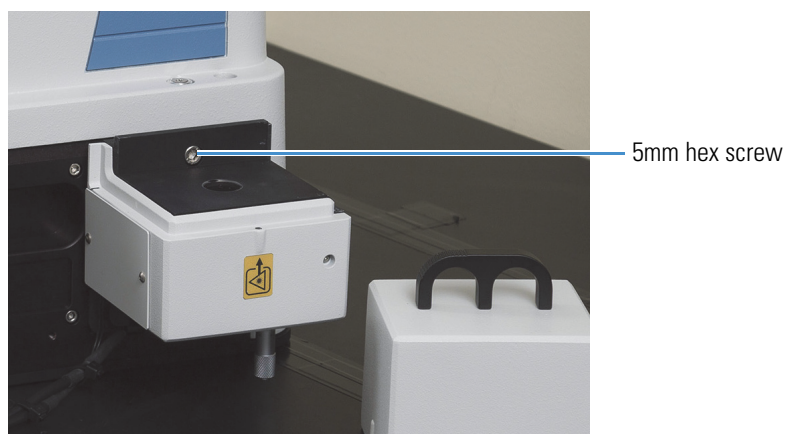


## Required Tools

- Hex driver, supplied.

### ❖ To install the iXR macro sampling accessory

1. Remove the top cover from the macro sampling accessory.
2. Using the guide pins on the accessory, mount the accessory over the laser output aperture on the instrument or on the camera body.
3. Using the supplied 5mm hex driver, mount the interface to the spectrometer or to the camera. The mounting plate attaches with two hex screws. One above and one below the lower sampling stage.



4. Connect the BNC cables to the laser interlocks. These prevent laser operation when the cover is removed.
5. Reinstall the accessory's top cover.

**Figure 10.** The macro sampling accessory shown installed and with the top cover on



## Maintenance and Storage

### Cleaning Your Instrument

If the outside of the instrument needs cleaning, turn off the power, unplug the power cable from the wall outlet, or power strip, and wipe the outside of the instrument with a damp (not wet), soft cloth and a mild soap. (Do not use harsh detergents, solvents, chemicals or abrasives.)



**WARNING** Avoid shock hazard. Do not allow liquid or any moist material to come in contact with the power supply or the inside of the instrument.

### Biohazards or Radioactive Materials and Infectious Agents

Instruments, accessories, components or other associated materials may not be returned to us or other accessory manufacturers if they are contaminated with biohazard or radioactive materials, infectious agents, or any other materials and/or conditions that could constitute a health or injury hazard to employees. If you have questions about decontamination requirements, [Contact Us](#).

### Replacing Fuses

You cannot replace the fuses in your instrument. If you suspect a fuse needs to be replaced, contact our sales or service representative in your area or visit our web site for assistance.

### Packing the Optional Shipping Case

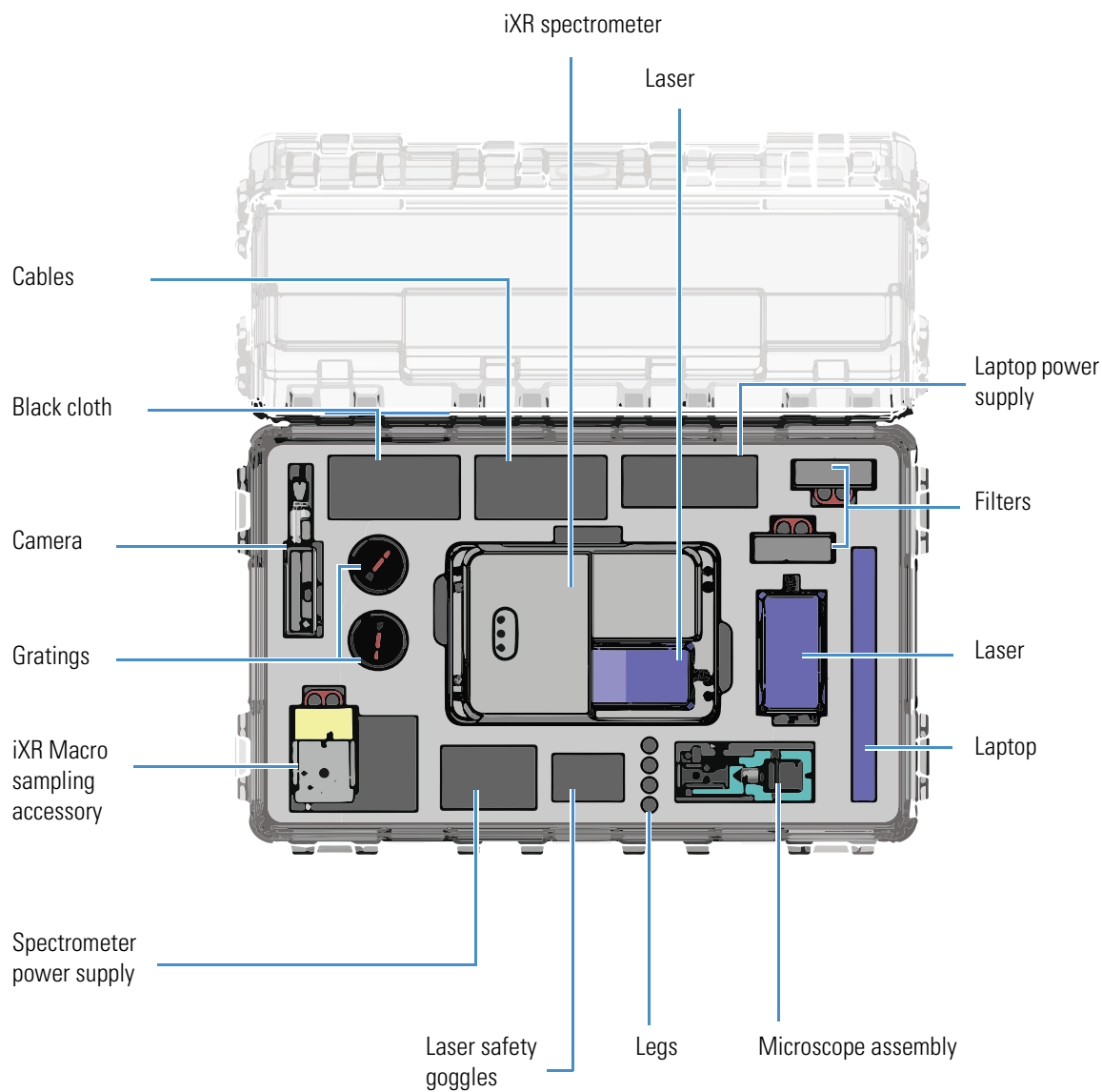
Before packing the spectrometer and any accessories in the optional shipping case, remove all accessories, laser, filter, grating, and legs.

**NOTICE** Humidity can damage optical components if they are not properly stored and protected. To protect components from humidity, anything with an optical component should be stored in a storage bag, including the following:

- The iXR spectrometer
- Microscope objectives
- Sampling accessories
- Laser, filter, and grating



**Figure 11.** Packing the optional shipping case



## Troubleshooting

If after following recommendations the problem persists, [Contact Us](#).

### Sample Bands are too Small

The Raman signal is too small. You can increase it by doing one or more of the following:

- Increase the setting of **Exposure Time** on the **Collect** tab.
- Increase the setting of **Exposures** on the **Collect** tab.
- Increase the aperture size by setting **Aperture** on the **Bench** tab.
- Select a slit aperture instead of a pinhole by setting **Aperture** on the **Bench** tab.
- Increase the setting of **Laser Power** on the **Bench** tab

**Note** All of the tabs mentioned here are in the **Experiment Setup** dialog box.

### Sample Bands Are too Large

The Raman signal is too large, which saturates the CCD. You can decrease the signal by doing one or more of the following:

- Decrease the setting of **Exposure Time** on the **Collect** tab.
- Decrease the aperture size by setting **Aperture** on the **Bench** tab.
- Select a pinhole aperture instead of a slit by setting **Aperture** on the **Bench** tab.
- Decrease the setting of **Laser Power** on the **Bench** tab.

**Note** All of the tabs mentioned here are in the **Experiment Setup** dialog box.

### No Raman Signal Appears in the Live Display

- Ensure all laser interlocks are properly closed
- Ensure the system is plugged in.
- If the laser power is off, turn on the laser.
- If the laser is disabled, enable it in the **Bench** tab of the **Experiment Setup** dialog box.
- Ensure the spectrometer cover is properly installed.
- Ensure that the sample interface is protected from the ambient light.

### **CCD Overflow Occurred**

Too much light hit the CCD. To correct this problem, try either of the following:

- Use a shorter exposure time or smaller aperture.
- Reduce the laser power.
- Ensure the spectrometer cover is properly installed.
- Ensure that the sample interface is protected from ambient light.

### **The Spectrum Has No Sample Bands**

- Ensure that the spectrometer cover is properly installed.
- Ensure that the sample interface is protected from ambient light.
- If the laser power is off, turn on the laser.
- If the laser is disabled, enable it in the **Bench** tab of the **Experiment Setup** dialog box.

### **The Spectrum Has Large Noise Spikes**

- Cosmic ray events occurred during data collection.
  - Turn on **Cosmic Ray Rejection** and set it to Medium. (**Cosmic Ray Rejection** is on the **Collect** tab of the **Experiment Setup** dialog box.)
- Ensure that the spectrometer cover is properly installed.
- Ensure that the sample interface is protected from ambient light.

### **The Spectrum Has a Sloping Background**

The sample may be fluorescing or heating. To account for this condition try one or more of the following:

- Correct the baseline to subtract the broad background.
- Use a different laser. Shorter wavelengths heat samples less.
- If the sample looks burned, replace it or move it so the laser will strike a fresh area.
- Reduce the laser power and collect the sample again. Watch the live display to see if the sample is still heating. (Reducing the laser power reduces the Raman signal generated at the sample and therefore the quality of the data. To compensate, try increasing the number of exposures or the exposure time.)

### **The Spectrum Baseline Is Severely Tilted or Curved**

The sample fluoresced during data collection. To correct this problem, try one or more of the following:



- Purify the sample.
- Make sure the sample container is not responsible for the fluorescence.
- If fluorescence is an inherent property of the sample, correct the baseline to subtract the broad background.
- Use a longer wavelength laser or expose the sample to the laser beam for a period of time before beginning the collection of the sample spectrum (this is known as “photobleaching”).
  - On the **Collect** tab of the **Experiment Setup** dialog box, turn on **Preview Data Collection** and type the desired exposure time in the **Preview Time** text box.

### **The Spectrum Baseline Has a Severe Positive Offset**

The sample is heating. To account for this condition try one or more of the following:

- Correct the baseline to subtract the broad background.
- Use a different laser. Shorter wavelengths heat samples less.
- If the sample looks burned, replace it or move it so the laser will strike a fresh area.
- Reduce the laser power and collect the sample again. Watch the live display to see if the sample is still heating. (Reducing the laser power reduces the Raman signal generated at the sample and therefore the quality of the data. To compensate, try increasing the number of exposures or the exposure time.)

### **The Spectrum Baseline Is Severely Shifted**

No background was subtracted from the sample data (the number of background exposures is set to zero or the Smart Background feature is disabled). The offset is the detector bias and dark signal. Set **Background Exposures** on the **Collect** tab of the **Experiment Setup** dialog box to an integer greater than 0.

### **A Grating Does Not Appear to Be Installed**

- Make sure a grating is installed.
- Exit Thermo Scientific™ OMNIC™ software, shut down the computer, turn off the instrument, wait 30 seconds, and then turn on the instrument.

### **A Laser Does Not Appear to Be Installed**

- Make sure a laser is installed and the keyswitch is turned on.
- Exit OMNIC, shut down the computer, turn off the instrument, wait 30 seconds, and then turn on the instrument.
- Make sure the spectrometer cover is properly installed.

### **A Filter or Fiber Optic Accessory Does Not Appear to Be Installed**

- Make sure a filter or fiber optic accessory is installed and properly seated.
- Exit OMNIC, shut down the computer, turn off the instrument, wait 30 seconds, and then turn on the instrument.

### **The Computer Cannot Communicate with the Instrument**

- Check the cable between the computer and the instrument. If it is disconnected, connect it.
- If the front panel indicators are not on, make sure the instrument is plugged in.

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