

NICOLET™ 8700
USB Version

User's Guide

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269-158600

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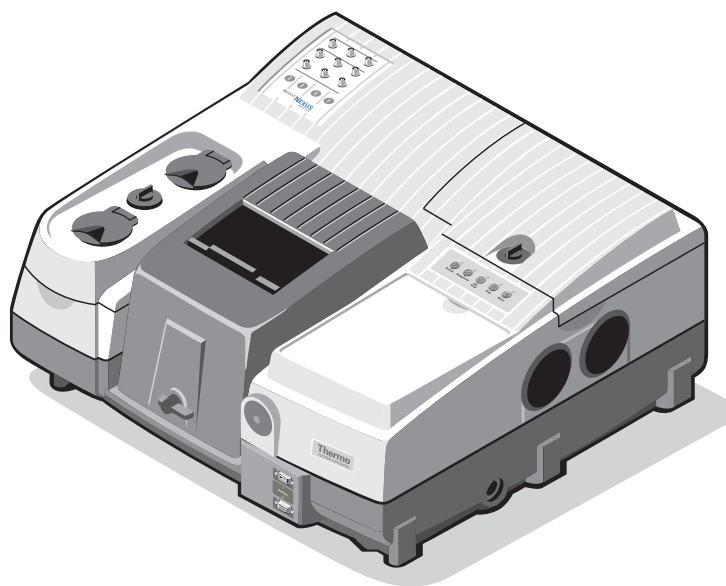
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Welcome

Congratulations on your purchase of a Nicolet™ 8700 USB version spectrometer from Thermo Fisher Scientific! The spectrometer lets you collect spectra in the mid-IR, far-IR and near-IR spectral ranges. It has all of the features of the other Nicolet FT-IR spectrometers, plus step-scan and dual-channel data collection and other advanced features. The system integrates advanced hardware features with the power and flexibility of OMNIC™ software.*



* Some dedicated systems use other Thermo Scientific software packages.



If you have not used the spectrometer before, view the “Spectrometer Tour” and “Getting Started with OMNIC” tutorials available through the OMNIC Help menu.

About this manual

This manual explains how to use the system to collect and process FT-IR spectra after the spectrometer is installed. Included is information about using your OMNIC software as well as chapters on how to operate, maintain and service the spectrometer.

This manual describes some hardware features that are not available on all Nicolet models. Use the instructions for the features on your system. Although the appearance of your spectrometer may vary from some of the illustrations in this manual, the instructions are correct for your system.

The following conventions are used in this manual to draw your attention to the on-line documentation and other important information.



This symbol tells you that you can find more information in the on-line tutorials and Help system. To access online information, click the Help menu in OMNIC. For questions about OMNIC SST software and experiments, click the SST menu in OMNIC and then choose SST Help.



This symbol tells you that you can find more information in a hardware or software manual that came with your system.

Note Notes contain helpful supplementary information. ▲

Notice Follow instructions labeled “Notice” to avoid damaging the system hardware or losing data. ▲

⚠ Caution Indicates a potentially hazardous situation which, if not avoided, may result in minor or moderate injury. It may also be used to alert against unsafe practices. ▲

⚠ Warning Indicates a potentially hazardous situation which, if not avoided, could result in death or serious injury. ▲

⚠ Danger Indicates an imminently hazardous situation which, if not avoided, will result in death or serious injury. ▲

Questions or concerns

In case of emergency, follow the procedures established by your facility. If you have questions or concerns about safety or need assistance with operation, repairs or replacement parts, you can contact our sales or service representative in your area or use the information at the beginning of this document to contact us.

Installing OMNIC

If you purchased your computer from Thermo Fisher, your software is already installed. If you provided your own computer, you need to install OMNIC on your hard drive. See the instructions that came with the software CD, or read “Installing OMNIC” in the document titled *OMNIC - Getting Started* that came with your software. You can use these same instructions if you ever need to reinstall the software.

Where to find the information you need

The on-line and printed documentation included with your system is designed to let you find the information you need quickly. We recommend first using the on-line documentation provided with OMNIC when you have a question. OMNIC includes several on-line tutorials, a wizard and a complete Help system. See “Starting OMNIC” in the “Before You Collect Spectra” chapter for information about starting OMNIC.

Wizards and tutorials

The following wizards and tutorials are available on your system.

Getting Started With OMNIC – This tutorial, available through Getting Started in the Help menu, introduces you to OMNIC. It includes basic information about the OMNIC window, using the toolbar and tool palette, creating and using spectral libraries, creating your own experiment files, and using on-line laboratory notebooks to create and save reports.

Spectrometer Tour – When you finish this tutorial, you will be familiar with the major components in your spectrometer. The tutorial is available through Getting Started in the Help menu.

Beginner’s Guide to FT-IR – Run this tutorial to learn how an FT-IR spectrometer works and the theory behind FT-IR spectroscopy. The tutorial is available through Getting Started in the Help menu.

Sampling Techniques – This item in the Help menu gives you access to the “Choosing a Sampling Technique” tutorial, which helps you choose the best technique for your analysis. Also available are tutorials describing how to install and use a number of sampling accessories, including Smart Accessories.

Learning OMNIC – This item in the Help menu gives you access to tutorials that explain how to use OMNIC to collect spectra and perform a number of other software operations.

Spectrometer Help Topics – This tutorial, available in the Help menu, contains step-by-step instructions for installing optional hardware, changing replaceable parts, maintaining your spectrometer, and setting up the system for a variety of experiments. If you ever have a problem with your spectrometer, use this tutorial to access troubleshooting information and get part number and ordering information.

Technical Support – This tutorial, available in the Help menu, outlines the many support, training, and custom application services available from Thermo Fisher. It includes Technical Support telephone and fax numbers, as well as e-mail and web site addresses.

The **Library Creation Wizard** prompts you, step by step, through creating a user library of spectra. The wizard appears when you click the Create Library button in Library Manager, available in the Analyze menu in OMNIC.

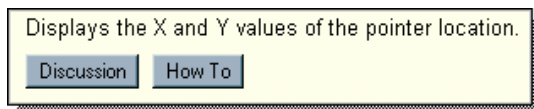
On-line Help

Choose the Help Topics that interest you from the Help menu to display that Help system. It lets you quickly find answers to your questions about using the software.

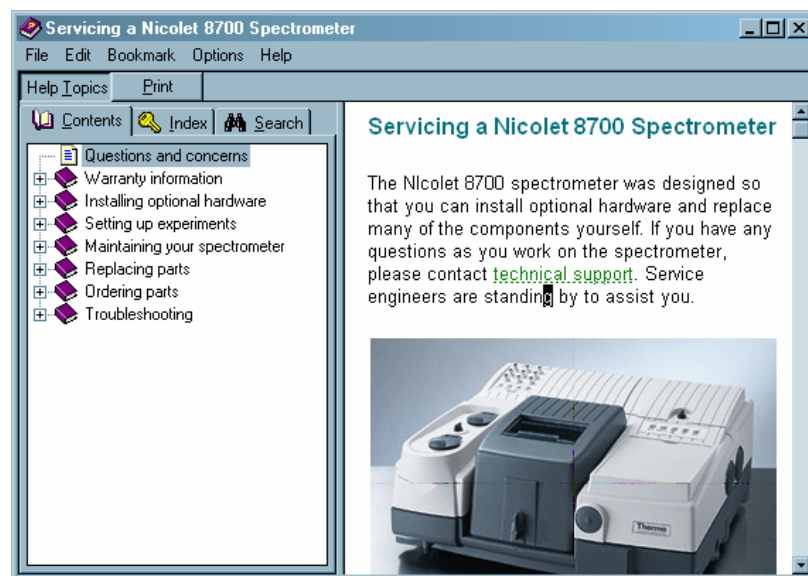
Additionally, you can find information about many features in your spectroscopy software (such as a parameter in a dialog box) by clicking the feature using the right mouse button.

If the active dialog box or window includes a question mark button near the upper-right corner, you may need to first click that button and then click the feature of interest using the left mouse button.

In either case, a brief description of the item appears, and in most cases buttons that allow you to access more detailed information. Here is an example:



Once the help system is open, the left pane in each help window lists the topics available in that help system. Here is an example of a help window showing the contents of some of the books in the system:



Advanced applications

Respected Thermo Fisher principal scientist Dr. Eric Y. Jiang's book *Advanced FT-IR Spectroscopy: Principles, Experiments and Applications Based on Research-Grade Nicolet FT-IR Spectrometers* has been made available through the SST menu. Choose Advanced Applications to access a wealth of theoretical background and application information.

Before You Collect Spectra

Warning

The *Spectrometer Safety Guide* that came with your system contains important safety information. This guide is available in several languages. Contact your local Thermo Fisher office for information about the languages that are available. Before you use the system, read the entire guide. To prevent personal injury and damage to equipment, follow the safety precautions contained in the guide whenever you use the system. ▲

Before collecting spectra check the following:

- Check the purge or desiccant.
- Make sure the system components are powered on.
- Cool the detector (if you are using an MCT, InSb or other detector that requires cooling).

Checking the purge

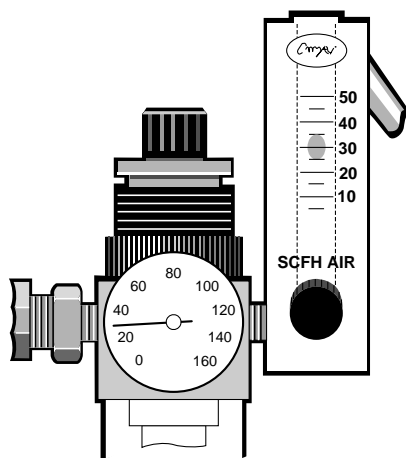
If your spectrometer is purged but you don't have the Smart Purge option, make sure the pressure regulator is set between 20 and 40 pounds per square inch (psi) and the flowmeter reads approximately 30 standard cubic feet per hour (scfh). The settings for systems equipped with Smart Purge are given in the next section; read this section first.



If you need to adjust the flow rate, or if your application requires a different flow rate, follow the instructions in “Setting the purge gas controls” in the “Setting up experiments” book in Spectrometer Help Topics.

Warning

Never use a flammable gas to purge the spectrometer. The purge gas must be free of moisture, oil, carbon dioxide and other reactive or infrared-absorbing materials. Use dried air or nitrogen to purge the spectrometer. Other gases, even inert gases such as argon, can damage the spectrometer and should never be used for this purpose. ▲



We recommend that you leave the purge on at all times. This keeps the spectrometer free of undesirable gases, protects the optics and improves the system's thermal stability.



In Spectrometer Help Topics view “Installing optional hardware” for information about installing purge equipment and setting the controls for the first time. “Maintaining your spectrometer” contains information about inspecting and replacing the purge filter. In the Spectrometer Tour (available through Getting Started) view “Sample compartment” for information about using Smart Purge.

Standard purge settings

For spectrometers that are equipped with standard purge, make sure the pressure regulator is set between 20 and 40 pounds per square inch (psi) and the flowmeter reads approximately 30 standard cubic feet per hour (scfh).



For more information about adjusting the pressure and flow rate, see “Setting the purge gas controls” in the “Setting up experiments” book in Spectrometer Help Topics.

Smart Purge settings

The Smart Purge option increases the purge gas flow rate when you install or remove samples. If you have this option, set the pressure regulator to 80 psi. The auxiliary tank may be required depending on the flow rate supplied by your purge gas source.

Flow Rate*	Tank Required?	Comments
less than 50 scfh	yes	Some purge gas and pure air generators provide a flow rate of less than 50 scfh.
50-99 scfh	optional	Using the tank will improve performance.
100 scfh or greater	no	A flow rate of 100 scfh gives the best results.

* Flow rates greater than 50 scfh cannot be measured with the flowmeter installed by Thermo Fisher. See your air dryer manual or contact the department that maintains your purge equipment if you don't know the flow rate of the purge gas source.



You can use OMNIC to set the duration of increased purge flow. In OMNIC Help Topics find “purge” in the Index and go to “Setting Smart Purge.”

Checking the desiccant



Check Desiccant...

If your spectrometer is sealed and desiccated, a bag of desiccant is located under the beamsplitter compartment cover. The desiccant protects the beamsplitter and other optical components by reducing the amount of water vapor inside spectrometer. See “Checking and changing desiccant” in the “Maintaining your spectrometer” book in Spectrometer Help Topics if you need to change the desiccant.

If your spectrometer is in use, check the humidity level inside it monthly (more often in very humid climates) by clicking the Check Desiccant button on the Diagnostic tab of the Experiment Setup dialog box. If the level exceeds the factory-specified limit, a message informs you. Be sure to change the desiccant so that the optics will be protected.



If your spectrometer is in storage, check the round, blue indicator on the desiccant holder under the beamsplitter compartment cover monthly. Change the desiccant if the indicator has turned pink. Keep all covers closed tightly while the spectrometer is in storage.

Note

The Check Desiccant button measures humidity more accurately than the indicator. For this reason you should rely on the button to monitor the performance of the desiccant when the spectrometer is in use. Rely on the indicator only when the spectrometer is in storage. ▲



See “Ordering parts” in Spectrometer Help Topics to find the part number for ordering desiccant bag.

Turning on the system components

We recommend that you keep your spectrometer on at all times, unless the building is subject to power outages or you need to perform a service or maintenance procedure. Leaving the system on keeps it stable and gives you the most consistent results. If you must turn the spectrometer off, allow it to stabilize for at least 15 minutes (one hour for best results) before collecting spectra.

Follow these steps to turn on the system components:

- 1. If the external power supply is not already connected, connect it.**



In the Spectrometer Tour (available through Getting Started) view “Connecting to AC power” in the “Powering up” unit for information about connecting the power supply.

- 2. Turn on any accessories you plan to use.**

This includes accessories such as a gas chromatograph (GC), PEM controller, electronic filters, an SSD demodulator or an infrared microscope.

Warning

Always follow the safety precautions described in this manual and in the *Spectrometer Safety Guide* that came with your system. ▲

- 3. Turn on the spectrometer by pressing the power switch (I/O) on the external power supply to I.**

When you turn on the spectrometer, the four status indicators—Power, Scan, Laser and Source—flash in various sequences as the system runs through its diagnostic routines. When the routines are finished, the Power, Laser and Source indicators stay lighted. The Scan indicator flashes with each scan of the interferometer.

After you turn on the spectrometer, let it stabilize for at least 15 minutes (one hour for best results) before collecting spectra.



See “Turning on the spectrometer power” in the “Spectrometer Basics” chapter if you need more information.

4. Turn on the printer and then the computer.

Turn on the printer and computer as explained in the documentation that came with those components.

Cooling a detector



Some detectors, such as an MCT or InSb detector, require cooling with liquid nitrogen or other cryogen. In Spectrometer Help Topics view “Cooling a detector” in “Setting up experiments” for instructions.

Warning

Liquid nitrogen is extremely cold and therefore potentially hazardous. Avoid contact with skin. Wear protective clothing and follow standard laboratory safety practices to prevent injury. Liquid nitrogen can be hazardous if handled in an insufficiently ventilated room. ▲

After you fill the detector dewar with liquid nitrogen (the dewar holds about 750 mL), allow the detector to cool at least 20 minutes before collecting spectra.



If you have not used the system before, you can familiarize yourself with OMNIC and the basic operation of the spectrometer by viewing the “Collecting a Spectrum” tutorial (available through Learning OMNIC in the Help menu) or by using the tutorial in the next chapter of this manual. These tutorials take you step-by-step through the process of collecting a simple transmission spectrum, allowing you to familiarize yourself with the spectrometer as you perform the experiment. If you need to change a source or detector, view “Replacing the source” or “Replacing the detector” in the “Servicing your spectrometer” book in Spectrometer Help Topics.

Note

A commonly used hardware configuration for mid-IR experiments includes a KBr beamsplitter, an ETC source and a DLaTGS detector. The example experiment sets the parameters for this hardware configuration. You may change the settings if your hardware configuration is different. ▲

Using Basic OMNIC Functions

This chapter introduces you to basic functions that allow you to collect and work with the data using OMNIC, including:

- Starting OMNIC.
- The OMNIC window.
- Using the data collection buttons.
- Using quality checks and status indicators.
- Saving a spectrum.
- Converting a spectrum to a variety of Y-axis units.
- Annotating spectra.
- Verifying the composition of the sample.
- Creating a user library.
- Adding a spectrum to a user library.
- Creating and printing a report containing spectra.

Follow the instructions in the preceding chapter to prepare the system and start OMNIC before using this chapter.

Note If you have a dedicated system (such as an ECO/RS) that normally uses a software package other than OMNIC, skip this chapter. See the special documentation that came with your system for instructions for using that software. If you need information about using the spectrometer, see the chapters that follow this one. ▲

Starting OMNIC

Follow these steps to start OMNIC:

1. Start your Windows® software.

Depending on the version of Windows you are using, you may be required to enter your user name and password. Enter the information when you are prompted.

2. Double-click the OMNIC shortcut on the Windows desktop.



Alternatively, you can click the Start button on the Windows taskbar, point to Programs (All Programs in Windows XP), point to the Thermo Nicolet folder, and then click the OMNIC program.

Depending on how the program has been configured, dialog boxes may appear asking for a user name and password. Type the requested information and then choose OK.



The OMNIC window appears. This window is described in the next chapter and in the “Getting Started With OMNIC” tutorial available through Getting Started in the Help menu.

OMNIC window

The large window that appears on the screen when you start OMNIC is called the OMNIC window.

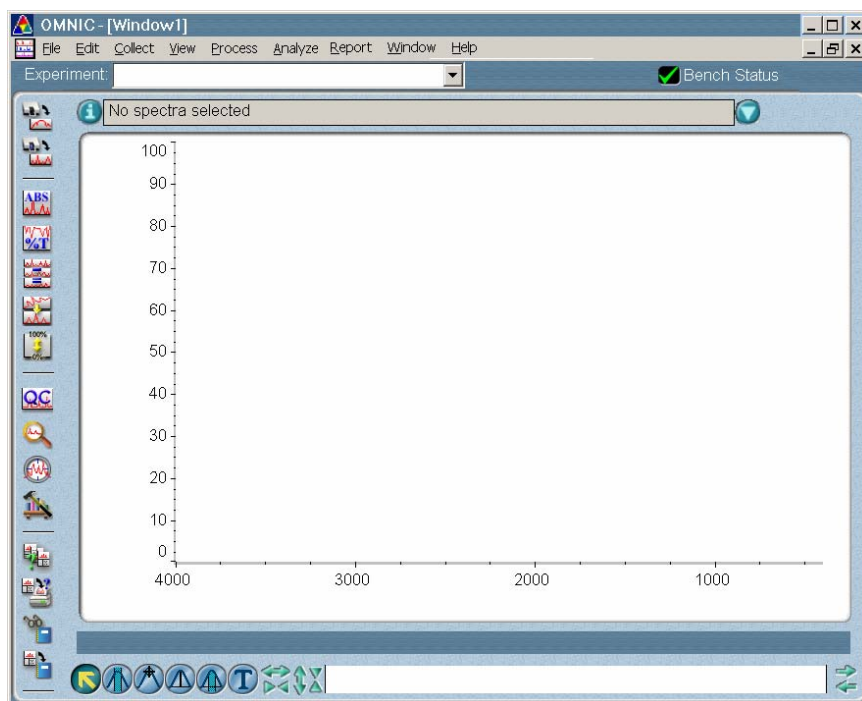
Menu bar

Below the title bar is the menu bar, which contains all of the OMNIC menu names. (Depending on which optional software you purchased, the menu names in your menu bar may be somewhat different from those shown.) Detailed information about the menu commands can be found in the on-line tutorials, the OMNIC Help system, or the OMNIC SST Help system.



Spectral window

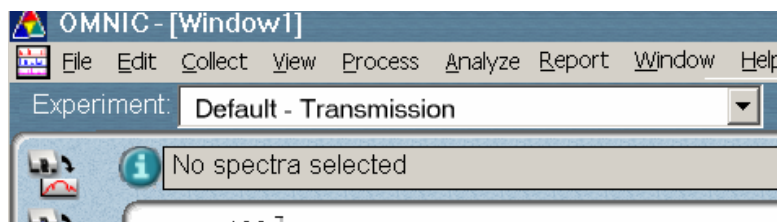
Within the OMNIC window is a spectral window, which you can use to display and manipulate spectra.



Experiment drop-down list box



Below the menu bar is the Experiment drop-down list box. It lists all of the experiment files you have opened, plus the default experiment file and an experiment file for any Smart Accessory module you have installed. By selecting an experiment with this feature, you can quickly set the software parameters for the type of experiment you want to perform. You can see the parameter settings for the selected experiment by using Experiment Setup, available in the toolbar or in the Collect menu.



Bench Status indicator

To the right of the Experiment drop-down list box is the Bench Status indicator.



If the indicator is a green check mark, the spectrometer has passed all of its diagnostic tests.



If the indicator is a yellow circle, a cooled detector in the spectrometer has become warm. A message appears explaining the problem and allowing you to access information about correcting it.



If the indicator is a red X, the spectrometer has failed a diagnostic test and requires corrective action. A message appears explaining the problem and allowing you to access information about correcting it.

Note If you wish to view the on-line videos while troubleshooting a problem, put the spectrometer's Tutorial CD into the computer's CD-ROM drive before selecting the video link. ▲



Toolbar

At the left side of the window is the toolbar. (You can use Edit Toolbar in the Edit menu to position the toolbar at the top or right side of the OMNIC window if you prefer.) Each button in the toolbar represents a command or other feature. To see the name of the command or feature, point to the button and wait a moment. To initiate the command or feature, click the button with the left mouse button.

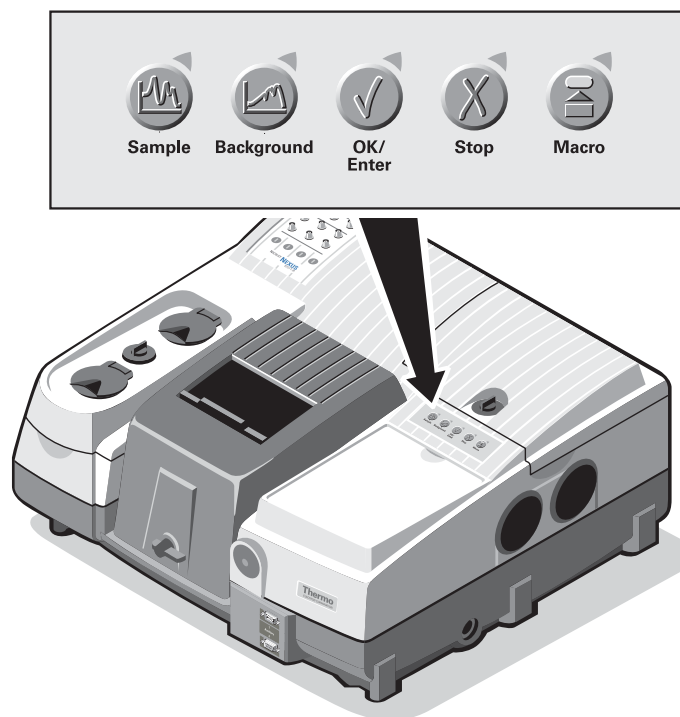


In OMNIC Help Topics find “toolbar” in the Index and go to “Displaying and using a toolbar” for information about using and customizing the toolbar buttons.

Note A commonly used hardware configuration for mid-IR experiments includes a KBr beamsplitter, an ETC (mid-IR to far-IR) source and a DLaTGS detector. You may need to change the settings of the example experiment if your hardware configuration is different. ▲

Using the data collection buttons

The buttons on the top of the spectrometer let you quickly perform some basic operations with the spectrometer without using your keyboard or mouse. (OMNIC must be running.)



Press the Sample button to collect a sample spectrum. This has the same effect as choosing Collect Sample from the Collect menu. In OMNIC Help Topics find “spectrum” in the Index and go to “Collecting a sample spectrum” for more information.



Press the Background button to collect a background. This has the same effect as choosing Collect Background from the Collect menu. In OMNIC Help Topics find “background spectrum” in the Index and go to “Collecting a background spectrum” for more information.



Press the OK/Enter button to respond affirmatively—for example, to a software prompt—during data collection. This has the same effect as choosing OK (or other affirmative response, such as Yes) within the software.

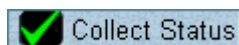


Press the Stop button to respond “Cancel” or “No” to a software prompt during data collection. This has the same effect as choosing Cancel or No within the prompt.



Press the Macro button to start a macro you have specified with the Macro for Macro button field on the Advanced tab in Experiment Setup. In OMNIC Help Topics find “macro” in the Index and go to “Specifying a macro for the Macro button” for more information.

How do I know if my spectrum is good?



The Collect Status indicator near the bottom of the Collect Sample window shows the status of the collection. When the indicator is a green check mark, it shows that the spectrum has passed all of the selected spectral quality checks made so far. After the collection is finished and the indicator is a green check mark, you can add the spectrum to a spectral window (if it is not added automatically).

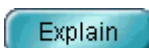
If you ever have a problem with data collection while one or more quality checks are turned on, the Collect Status indicator may change.



If the indicator is a yellow circle, the spectrum has failed a spectral quality check (a measured value was not within the allowed range), but it is not serious enough to stop the collection.



If the indicator is a red X, there is a problem with the quality of the spectrum. After correcting the problem, collect the spectrum again.



To view information about the collection, including a list of any problems that have occurred, click the Collect Status indicator during or after the collection. You can also click the View Collect Status button in the message that may appear when the collection is finished (see step 7 of the procedure in the preceding section). For each listed problem, an Explain button is provided to let you access troubleshooting information.

Saving a spectrum

You can save your spectrum on the hard disk by using either of two commands in the File menu: Use Save when you want to save a spectrum using the current filename and path. Use Save As when you want to save a spectrum using a new filename or path.

Converting Y-axis units

FT-IR spectra can be displayed as functions of intensity of energy transmitted, reflected, or absorbed plotted against the frequency at which the absorption, reflection, or transmission occurs. % Transmittance and % Absorbance are common units. The OMNIC toolbar includes buttons that allow you to easily convert from one y-axis unit to another.



Since many of OMNIC's data manipulation commands work best on spectra displayed in absorbance units, it is often useful to convert a spectrum to absorbance by using the Absorbance button. You also can choose Absorbance from the Process menu



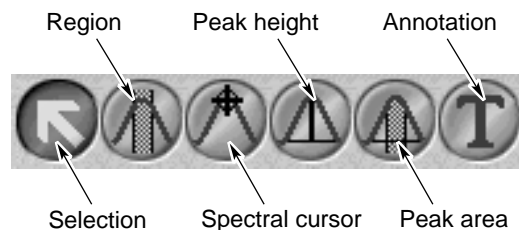
The data can be returned to % Transmittance by clicking the %T button. You also can choose % Transmittance from the Process menu.



The Process menu allows you to convert spectra to several other units, including Kubelka-Munk, photoacoustic, % Reflectance and $\log(1/R)$. These units are discussed in detail in the OMNIC on-line Help system. In OMNIC Help Topics find “converting spectrum” in the Index and go to the topic that deals with the units you are interested in.

Annotating spectra

The palette contains six tools that let you select a spectrum or spectral region, change how spectra are displayed in a spectral window, find the height or area of a peak, or label a peak. The names and appearance of the palette tools indicate their functions.



Only one tool can be used at a time. To use a tool, first select it by clicking it. A tool remains selected until you select another tool.

When you use a tool, the readout above the palette may display information for the tool operation, such as the X and Y values of the pointer location or the limits of the selected spectral region. Here is an example of X and Y values displayed in the readout when the selection tool is selected and the pointer is within the spectral display:

X: (3427.273) Y: (2.504)



The annotation tool lets you label peaks with their frequency locations (X values) or other information.

When the annotation tool is selected and you move the pointer into the spectral display, the pointer looks like this:



You can label a peak by clicking above it with the annotation tool. This displays the label text above the peak with a line connecting the label to the peak. The text is selected so that you can immediately edit it. When you press Enter, the label appears in its final form. You can more accurately locate the top of a peak by holding down the Shift key when you click near the peak. Press Enter to accept the label text.

You could also perform other operations on the label using the annotation tool. To modify a newly created label, edit the selected text before pressing Enter. To modify an existing label, click it and then type a new label and press Enter. To delete an existing label, click it and then press the Delete key.



In OMNIC Help Topics find “tool, annotation” in the Index and go to “Annotation tool” for more information about the annotation tool.

Verifying the composition of the sample

You can verify the composition of your polystyrene sample by automatically comparing the collected spectrum with the spectra in a QC (Quality Control) library. The software compares the sample spectrum with reference spectra in the appropriate category in the library and then tells you whether the sample matches a library spectrum.

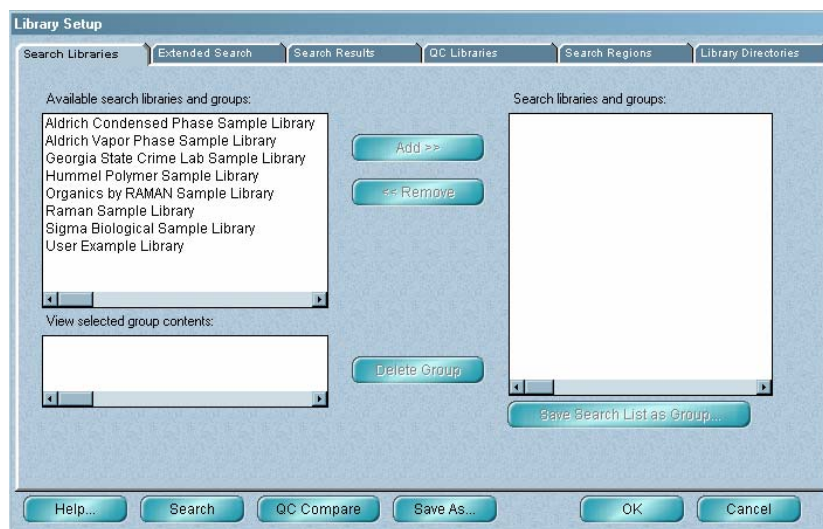
Note If you were unsure of the composition of the sample, you could perform a “spectral search” using a search library. In that case, the software would search the library and then display a list of the library spectra that best matched the unknown spectrum. ▲

Follow these steps to perform a QC comparison:

- 1. Select the spectrum by clicking it.**

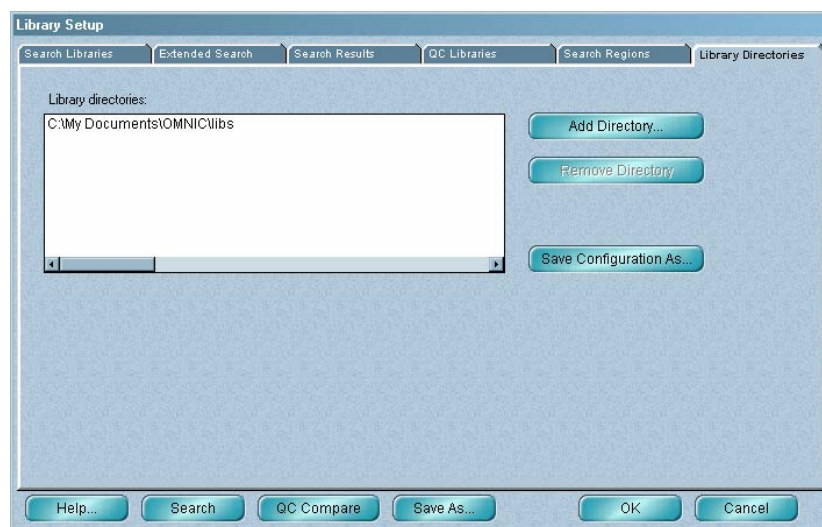
2. Choose Library Setup from the Analyze menu.

The Library Setup dialog box appears:



3. On the **Library Directories** tab, add the **LIBS** directory (within the **OMNIC** directory) to the list of directories in the **Library Directories** box if it is not already in the list.

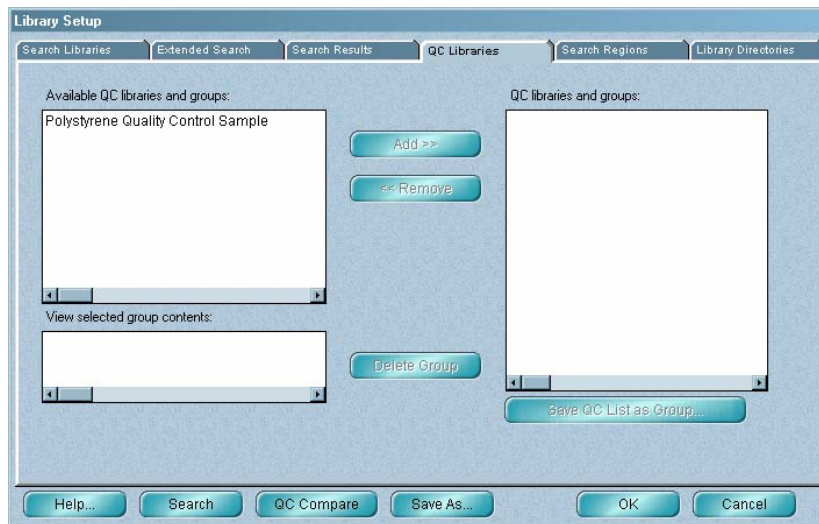
The Library Directories box lists the directories that are currently being used for spectral searches and QC comparisons. All the libraries in the listed directories are available for your QC comparison.



The LIBS directory contains the provided Polystyrene Quality Control Sample library. To add the directory to the list, choose Add Directory. In the dialog box that appears, locate and select the LIBS directory, and then choose OK.

4. Click the QC Libraries tab to display the available QC libraries.

The available QC libraries appear in the Available QC Libraries And Groups box.



The libraries listed in the QC Libraries And Groups box are the libraries with which your spectrum will be compared.

5. Add the Polystyrene Quality Control Sample library to the comparison list.

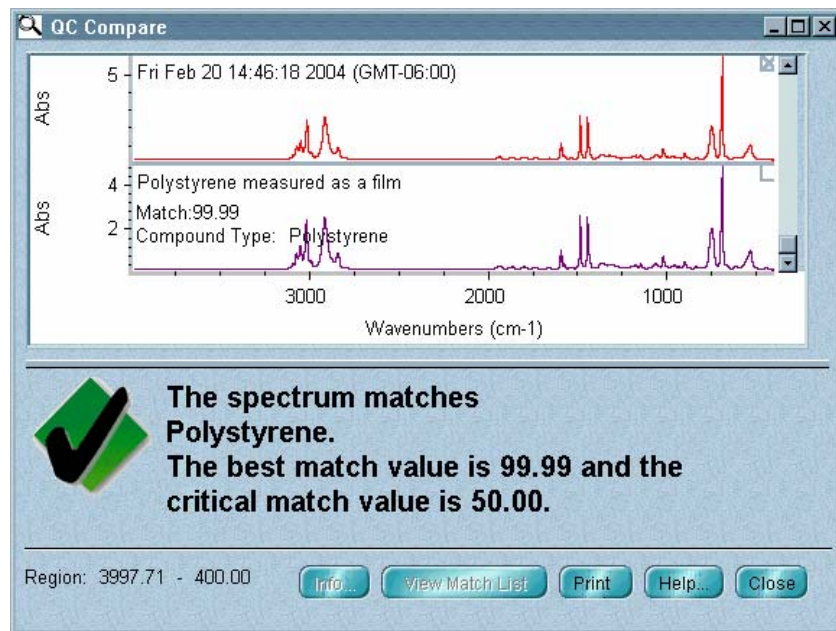
To do this, click the appropriate library name in the Available QC Libraries And Groups box, and then click the Add button.

6. Choose QC Compare in the Library Setup dialog box to start the comparison.

You can also close the Library Setup dialog box and begin a QC comparison at any time by choosing QC Compare from the Analyze menu.

When you begin a comparison, the QC Compare window appears. At the bottom of the window a gauge shows the progress of the comparison.

When the comparison is finished, the sample spectrum and the library spectrum that best matches it are displayed in panes in the upper portion of the window. Comments about the comparison appear in the lower portion of the window. Here is an example:



7. Close the QC Compare window by choosing Close.



In OMNIC Help Topics find “QC comparison” in the Index and go to “Performing a QC comparison” if you want more information about comparing sample spectra with QC libraries.

If you are using OMNIC, start the Library Creation Wizard by choosing Library Manager from the Analyze menu and then clicking the Create Library button on the Library Names tab.



In OMNIC Help Topics find “library, creating” in the Index and go to the “Creating a user library” topic for more information.

Adding a spectrum to a user library

Once you have created a user library, you can use the library to store spectra you have collected. To do this, select the spectrum and then choose Add To Library from the Analyze menu. To move a copy of a spectrum you have collected from one user library into another, use Library Manager in the Analyze menu.

Note You cannot add spectra to a commercial library, nor can you move copies of commercially collected reference spectra into libraries you create. ▲



In OMNIC Help Topics find “adding, spectrum to user library” in the Index and go to the “Adding a spectrum to a user library” topic or the “Adding user library spectra to another user library” topic for more information.

Creating and printing a report



OMNIC makes it easy to create and print a report containing the results of your work.

You can also view the “Creating Reports” tutorial (available through Learning OMNIC in the Help menu) to learn how to create and print reports and add them to report notebooks.

To create and print a report:

1. Choose Template from the Report menu.

A dialog box appears allowing you to select a report template for the report.

2. Select the report template file named QCCOMP.RPT.

This file contains a report template specially set up for this procedure. The template has items for the spectral window, spectrum time, title and comments, and QC comparison results.

When you select the template file, a preview image of the template appears at the right. This feature allows you to see what different templates look like so that you can pick one with the items you need for your report. You can view the image as a graphical layout by selecting the Layout option. This shows you how the printed report will look on paper. You can also view the image with template items labeled by selecting the Description option. This lets you identify items that are too small to be seen clearly.

3. **Choose Select to make the example template the current template for printing reports.**

When you print your report, OMNIC will automatically fill in the items in the template with the appropriate information and images. For example, if an item in the template is linked to the active spectral window, the contents of that window are included when you print the report.

You can create your own report templates by using the Create button, or you can modify one of the existing templates whenever you want to design a new template. Save the template with a new name after you make your changes

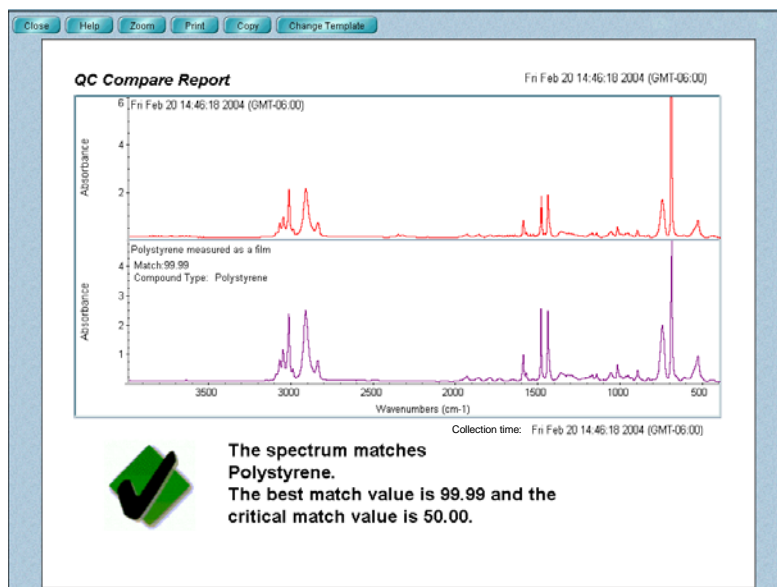


In OMNIC Help Topics find “report template, selecting” in the Index and go to “Selecting, editing or creating a report template” for more information about using reports.

4. **Choose Preview/Print Report from the Report menu.**

A preview of the report appears showing the report items filled in with information about your spectrum. The preview lets you check the content of the report before printing it.

Your report should look similar to this:



You can click the Zoom button to see an enlarged image of the report.

5. **If you have a printer connected to the computer, choose Print to print the report.**

The Print dialog box appears allowing you to set some parameters that affect printing.

6. **Choose OK to print the report to the default printer or, if you wish to print to a different printer, select it and then choose OK.**

Using the SST Software

The SST menu in OMNIC gives you access to the SST experiments that are available on your system.

On-line Help for SST

You can access on-line Help for the SST software by choosing SST Help from the SST menu. Also, if you press the F1 function key while you are in any SST dialog box or window or while any SST menu command is highlighted, the on-line Help information for that item appears.

Collecting data with SST

You can use the commands in the SST menu to collect sample and background data.

To collect SST data:

- 1. Choose the technique you wish to use from the SST menu.**

The menu lists the experiments that are available for your spectrometer.

- 2. When the setup dialog box for the SST technique appears, set the parameters for your experiment.**

Note If you change the spectral resolution, points before ZPD, or sample spacing parameters using one of the SST setup screens, it overwrites the same parameter for all SST and standard OMNIC data collection modes. ▲

3. **When the software is set up for your experiment, choose OK.**

You are returned to OMNIC.

4. **Use the commands in the SST menu to collect your background or sample data.**

Ratioing spectra

The Ratio Spectra command in the SST menu allows you to perform spectral division, ratioing any one spectrum or a group of three or more spectra against a common background spectrum. The background spectrum must be stored on a disk. You may also ratio two active spectra against each other.

Note

Whenever you ratio spectra, all of the spectra you select must be in the same final format, typically single beam. For example, you cannot ratio an absorbance spectrum against a transmittance spectrum. ▲

Ratioing spectra against a common stored background

Follow these steps to generate a ratioed spectrum from a stored background:

1. **Open a single-beam spectrum.**

If you wish to ratio a group of single-beam spectra, open all of the spectra into one spectral window.

2. **Select the spectra you wish to ratio.**

3. **Choose Ratio Spectra from the SST menu.**

The Ratio Spectra dialog box appears.

4. Select the background spectrum to be used as the denominator.

Use the Browse button to locate and select a background spectrum that you previously saved on a disk.

5. Select the destination for the ratioed spectra.**6. Choose OK to generate the ratioed spectrum.**

The results of the ratio operation appear in the window you specified as a destination.

Note Choose Cancel to exit the dialog box without ratioing the spectra. ▲

The special case of ratioing only two spectra

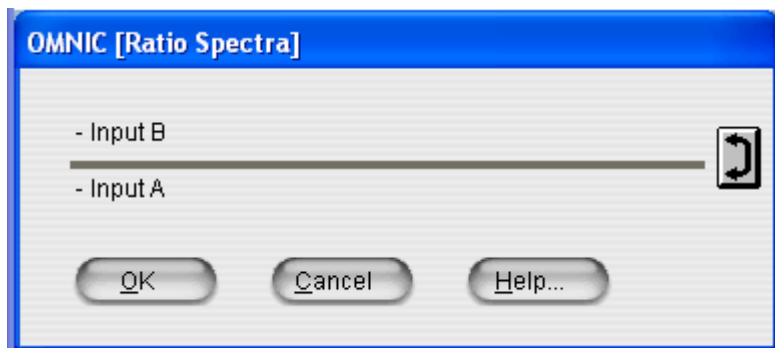
When you use the Ratio Spectra command with only two single-beam spectra selected, the command operates a bit differently. It generates a ratioed spectrum from those spectra. In this case, you do not have the opportunity to select a stored background spectrum. If you need to ratio only two spectra against a stored background, ratio each of them separately.

Follow these steps to generate a ratioed spectrum from two selected spectra:

1. Open and select the two single-beam spectra you wish to ratio.

2. Choose Ratio Spectra from the SST menu.

The Ratio Spectra dialog box appears.



3. If the spectra are not correctly positioned as numerator and denominator, click the Swap button at the right.

4. Choose OK to generate the ratioed spectrum.

Choose Cancel to exit the dialog box without ratioing the spectra.

The results of the ratio operation appear in the spectral window.

Using SST phase array operations

Phase array operations offer stored phase correction that lets you reprocess (using the commands in the OMNIC Process menu) spectra collected using step-scan PM, step-scan SMM, dual channel, and other experimental techniques that generate two or more spectra from the same scan. You can also use them to view and manipulate phase correction arrays for other spectra

What is a phase array?

A phase array is a frequency-dependent list (or spectrum) of phase angles calculated from the Fourier transform of an interferogram truncated around the ZPD. Each phase angle in the array is defined by the following equation:

$$\Phi_i = \arctan \frac{I_i}{R_i}$$

where I_i and R_i are the imaginary and real points from the Fourier transform at frequency i .

The phase array is used to correct the full-resolution single-beam spectrum for phase shifts caused by optical differences in the beamsplitter substrate and the compensator plates and for the probability that the central peak maximum point is not at exactly the zero-path-difference (ZPD) point.

What is phase correction?

Phase correction is one of several operations performed on the raw data collected by the detector. During the Fourier transform of an interferogram to a spectrum that can be analyzed, an apodization function, a zero filling factor, and a phase correction method must be used.

The phase correction is calculated using the following formula:

$$X_i = R_i \cos\theta_i + I_i \sin\theta_i$$

where R_i and I_i are the real and imaginary points from the Fourier transform of the entire interferogram at frequency i , θ_i is a phase angle from the phase array (interpolated, if necessary), and X_i is the single-beam spectrum.

In some experiments, such as step-scan multiple modulation and step-scan time-resolved, more than one interferogram is collected during a single scan. To obtain valid data from these experiments, a single phase correction array must be used for all the interferograms collected during the scan.

When you use the Collect Sample command in the SST menu, this is handled automatically by the OMNIC SST software. When you reprocess the data, the OMNIC software must be directed (using the Phase Array Operations command in the SST menu) to use the same phase correction array for all of the interferograms. If you do not direct OMNIC to use a stored phase array, a new phase array is calculated from each interferogram.

Phase array operations

The Phase Array Operations command in the SST menu lets you calculate, store and use a stored phase array for correcting any spectrum. You can also examine and manipulate the phase array used for the correction. This is useful when you need to apply different Y-axis constraints to the phase array.

Calculating a phase array

Follow these steps to calculate a phase array.

1. Save the interferograms when you collect the data.

There are two options for saving interferograms.

You can turn on Save Interferograms before beginning data collection. This option is in the File Handling box on the Collect tab in the Experiment Setup dialog box.

You can select Interferogram as your final format. The Final Format parameter is on the Collect tab in the Experiment Setup dialog box.

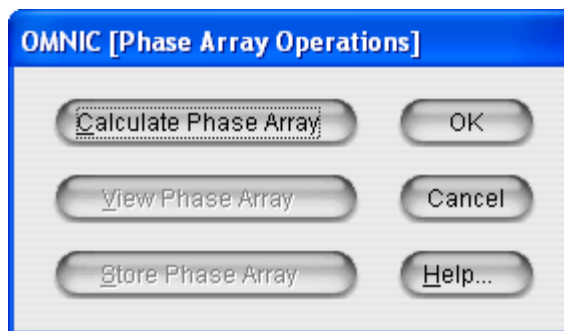
2. Open and select the interferogram.

If you chose to save the interferograms with your spectrum, use Open in the File menu to display the spectrum in a spectral window. Choose Reprocess from the Process menu. Select Interferogram from the Final Format drop-down list box. Choose OK. The interferogram appears in a spectral window.

If you selected Interferogram as your final format, the interferogram will be displayed automatically when data collection is finished. If the interferogram is already saved, use Open in the File menu to display the interferogram in a spectral window. The interferogram is selected automatically.

3. Choose Phase Array Operations from the SST menu.

The Phase Array Operations dialog box appears.



4. Choose Calculate Phase Array.

5. Choose OK.

Viewing a phase array

You must calculate the phase array before you can view it.

Follow these steps to view a phase array:

1. Choose Phase Array Operations from the SST menu.

The Phase Array Operations dialog box appears.

2. Choose View Phase Array.

The phase array appears in the active spectral window. You can manipulate it using the commands in the Process menu. You can then store the modified phase array and use it to generate spectra. Refer to the OMNIC Help system if you are unfamiliar with the Process menu commands.

Storing a phase array You must calculate and view the phase array before you can store it.

Follow these steps: to save a phase array:

1. Select a phase array.

2. Choose Phase Array Operations from the SST menu.

The Phase Array Operations dialog box appears.

3. Choose Store Phase Array.

The phase array will then be stored in memory and can be used to process subsequent interferograms.

4. Choose OK to close the dialog box.

Note If you calculate and store a new phase array, the new phase array replaces any phase array currently in memory. Only one phase array can be stored at a time. ▲

Note When a phase array is stored, you can use it to process (Fourier transform) an interferogram with the Store Phase option in the Reprocess dialog box. ▲

Saving a phase array OMNIC SST stores phase arrays as standard OMNIC spectral data files. Once you have saved an array, you can open it using any program that can read OMNIC files.

Note You must calculate and view a phase array before you can save it. ▲

To save a phase array follow these steps:

- 1. Select a phase array.**
- 2. Use the Save As command in the File menu and save the phase array.**

You will be prompted for a filename and directory path. Refer to the OMNIC Help system and your Windows documentation if you are unfamiliar with naming and saving files.

Spectrometer Basics

This chapter describes the major components of your Nicolet 8700 spectrometer, including the light source, beamsplitter and detector. It then explains what you need to know before collecting data in various spectral ranges.



In the Spectrometer Tour (available through Getting Started) view “From the front,” “The back panel” and “Inside the spectrometer” for complete descriptions of your spectrometer’s internal and external components.

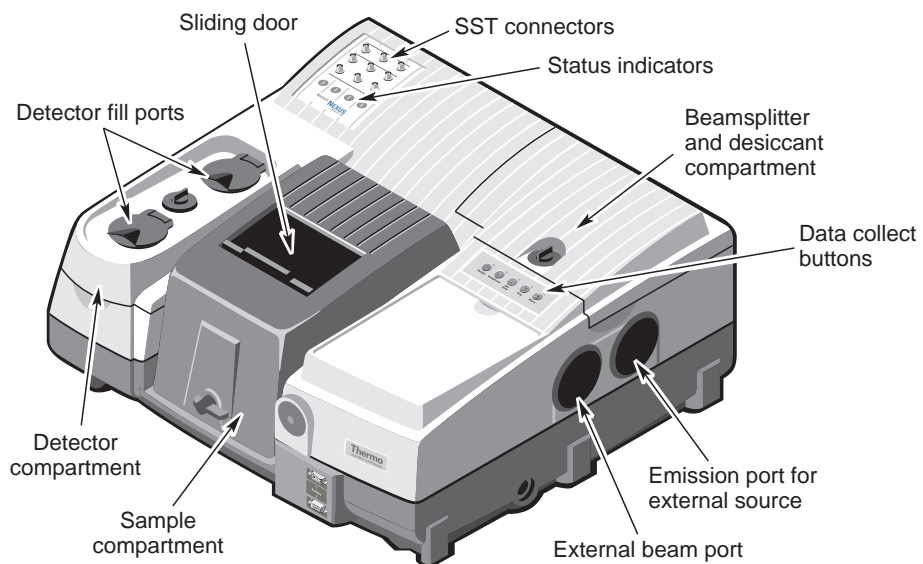
Spectrometer components

The following illustration identifies some major components visible on the outside of a typical Nicolet 8700 spectrometer. (Some components may not be present on your spectrometer.)



In the Spectrometer Tour (available through Getting Started) view “From the front,” “The back panel” and “Inside the spectrometer” for complete descriptions of your spectrometer’s internal and external components.

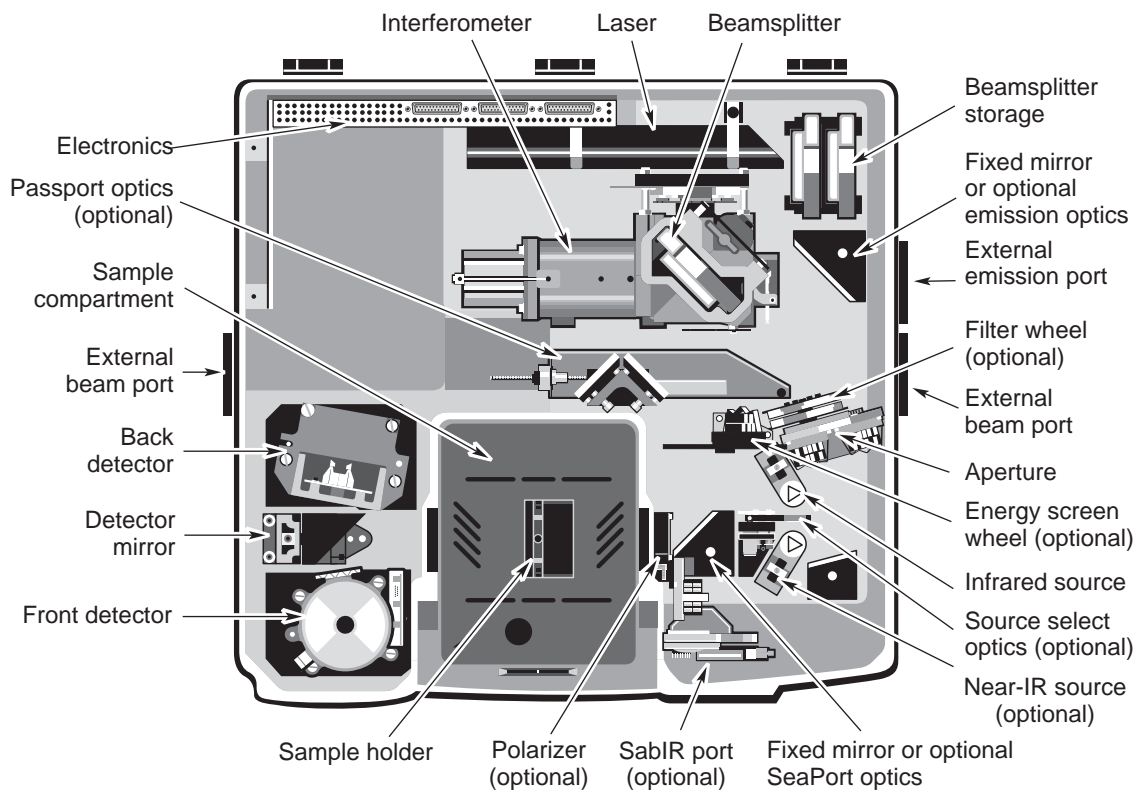
From the outside



Choose SST Help Topics from the SST menu to find complete information about using the SST connectors.

What's inside?

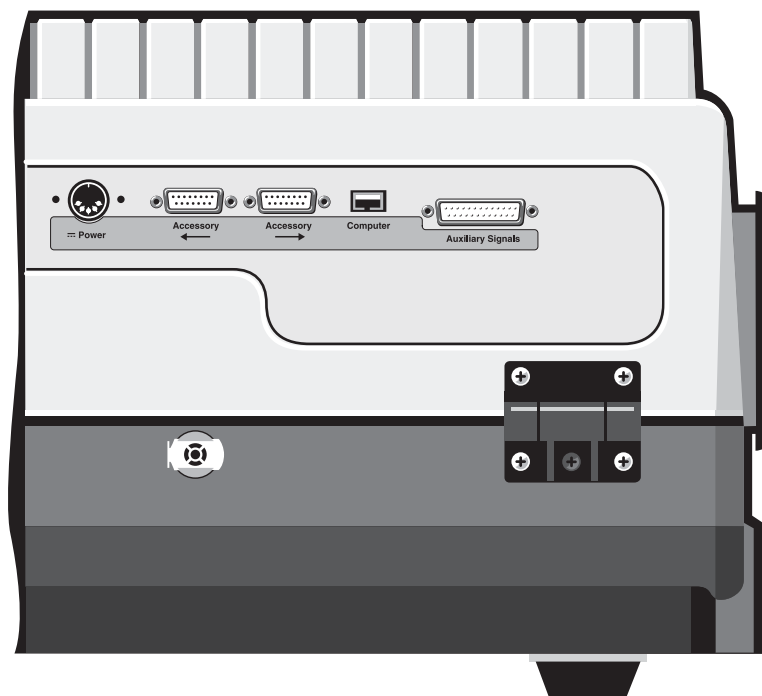
The illustration below shows a top view of the optical layout of the spectrometer with covers removed to reveal components.



In the Spectrometer Tour (available through Getting Started) view “Inside the spectrometer” for complete descriptions of your spectrometer components.

What's on the rear panel?

The illustration below shows the locations and uses of the connectors on the spectrometer rear panel:



In the Spectrometer Tour (available through Getting Started) view “The back panel” for complete descriptions of the rear panel components.

⚠ Danger

Avoid shock hazard. Always power off the spectrometer and disconnect the power supply from the wall outlet or power strip before disconnecting the power supply from the back of the spectrometer. ▲

⚠ Warning

Improper or unsafe cabling can cause damage to system hardware and may create a safety hazard. Thermo Fisher is not responsible for damage or injury resulting from improper or unsafe cabling. ▲

For more information about the Auxiliary pass-through connectors, see the “How to cable an accessory” section of the “Accessories” chapter.

Powering on

Follow these steps to turn on the spectrometer power:

1. **If the external power supply is not already connected, connect it.**



In the Spectrometer Tour (available through Getting Started) view “Connecting to AC power” in the “Powering up” unit for information about connecting the power supply.

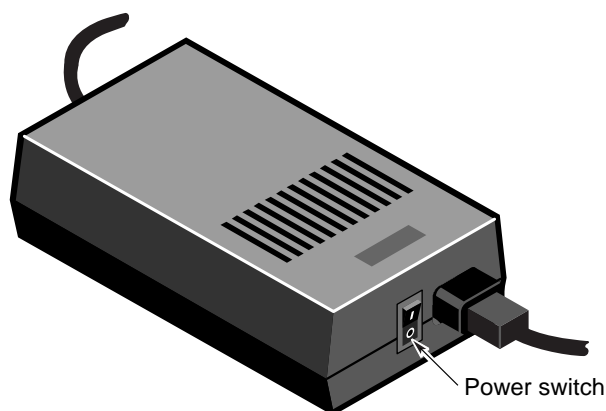
2. **Turn on any accessories you plan to use.**

This includes accessories such as a gas chromatograph, a PEM controller, an SSD demodulator or an infrared microscope.

Warning

Always follow the safety precautions in this manual and in the *Spectrometer Safety Guide* that came with your system whenever you use the spectrometer. ▲

3. Turn on the spectrometer by pressing the power switch (I/O) on the external power supply to I.



When you turn on the spectrometer, the four status indicators—Power, Scan, Laser and Source—flash in various sequences as the system runs through its diagnostic routines. When the routines are finished, the Power, Laser and Source indicators stay lighted. The Scan indicator flashes with each scan of the interferometer.

If the Power, Laser or Source indicators flash or will not light at all, or if the Scan indicator will not light, the Bench Status indicator will show a red X and troubleshooting tips will appear on the screen. If you cannot resolve the problem by following these tips or by turning the spectrometer power off and then on, contact technical support.

Note After you turn on the spectrometer, let it stabilize for 15 minutes (one hour for best results) before collecting data. Leave the spectrometer on at all times, unless the building is subject to power outages or you need to perform a service or maintenance procedure. Leaving the spectrometer on increases stability and consistency of performance. ▲

The spectrometer enters a “long-stroke” mode 10 minutes after data collection activity has ceased. This mode continues for 1 hour. If the source was in Turbo mode, it switches to Normal mode. After 1 hour, the interferometer stops scanning and the Scan light stays on. At this point, the source is put into Rest mode. Any data collection activity will cause the interferometer to begin scanning with the source in Normal mode. Exiting OMNIC also activates the long-stroke mode and moves the source from Turbo to Normal mode.

4. **Turn on the printer and then the computer.**

Turn on the printer and computer as explained in the documentation that came with those components.



In the Spectrometer Tour (available through Getting Started) view “Powering Up” for complete instructions on turning on your system.

Using a light source

The Nicolet 8700 has an IR source and a near-IR source. You can switch between different internal sources simply by changing the Source setting on the Bench tab of the Experiment Setup dialog box. This option lets you collect spectra in the mid-IR to far-IR range or in the visible to near-IR range. The spectral range is determined by the source, beamsplitter and detector you are using.



In Spectrometer Help Topics view “Installing a new source” in “Setting up experiments” if you need to install or change a source.



Caution

Even after the spectrometer is turned off, the external housings of working IR sources remain hot for up to 15 minutes. To avoid being burned, allow the source to cool before touching it. ▲

The ETC infrared source can be operated in the three modes of operation described below.

Normal mode – In this mode the temperature of the source is maintained at an optimal level for normal spectral data collection. This improves the consistency of your spectral data by ensuring that the infrared energy level reaching your samples is constant. The source operates in Normal mode unless you configure it to enter Turbo or Rest mode at specific times or the spectrometer is in sleep mode.

Turbo mode – Use this mode if you are analyzing a sample, such as a thick film, that requires greater infrared energy. This increases the output of the source, especially in the frequency range around 2,500 wavenumbers. To turn Turbo mode on or off, use the Source parameter on the Bench tab of the Experiment Setup dialog box, available through Experiment Setup in the Collect menu. So long as you are collecting data, the source remains in Turbo until you turn that mode off. Whenever the spectrometer is in stand-by mode, the source returns to Normal mode. When the spectrometer enters sleep mode, the source shifts into Rest mode. This extends the life of your source. In OMNIC Help Topics find “source” in the Index and go to “Specifying the source type” for details.

Rest mode – Rest mode lowers the temperature of the source so that its life is extended. The source automatically shifts into Rest mode when the spectrometer moves into sleep mode. You can configure the source to enter Rest mode at specific times.

The image shows a software dialog box titled "Source Rest Mode". It contains the following elements:

- An unchecked checkbox labeled "Inactivity Rest mode".
- A text input field labeled "Hours of inactivity:" with the value "0".
- An unchecked checkbox labeled "Daily Rest mode".
- A text input field labeled "Exit Rest mode:" with the value "12:00 AM".
- A text input field labeled "Start Rest mode:" with the value "12:00 AM".
- A section labeled "Rest days:" with seven checkboxes corresponding to the days of the week: Su, Mo, Tu, We, Th, Fr, and Sa. All checkboxes are currently unchecked.

When you resume data collection activity, the source automatically reenters Normal mode. In OMNIC Help Topics find “source” in the Index and go to “Extending the life of the source with rest mode” for details.

You can switch between different internal sources simply by changing the Source setting on the Bench tab of the Experiment Setup dialog box. This option lets you collect spectra in the mid-IR to far-IR range or in the visible to near-IR range. The spectral range is determined by the source, beamsplitter and detector you are using.

Nicolet 8700 spectrometers with the emission accessory can use an external source, if one is available. The beam from the external source passes through the emission port on the right side of the spectrometer.



In OMNIC Help Topics find “source” in the Index and go to “Specifying the source type” for instructions for using different sources in your spectrometer.

Selecting the right detector, source and beamsplitter

A number of light sources, beamsplitters and detectors are available for use in the Nicolet 8700 spectrometer. While you can change both the detector and beamsplitter types, you should be aware that not all beamsplitters and detectors can be used together. Also, some detectors can accommodate only a portion of the energy from the source and require changing the aperture size or installing an energy filter. This section explains how to select and optimize the performance of beamsplitters and detectors.



In Spectrometer Help Topics view the appropriate lesson in “Setting up experiments” if you need to install or change a beamsplitter or detector.

There are two considerations when selecting a beamsplitter-detector combination: compatibility and spectral range. Combinations are considered compatible if they provide a detector signal that is large enough to allow the beamsplitter to be aligned. This does not necessarily mean a particular combination will provide the maximum capable sensitivity range of each component.

The following table shows the beamsplitter-detector-source combinations are available and lists the spectral range for each combination. Note that the visible spectral range is based on aluminum optics used in the spectrometer.

Light Range	Beamsplitter	Detector	Spectral Range (cm ⁻¹)	Source
UV/visible	quartz	PbSe	13,000 - 2,800*	ETC, white light
		Si [†]	27,000 - 8,600	white light
	CaF ₂	PbSe	13,000 - 2,000*	ETC, white light
		Si [†]	14,500 - 8,600	white light
near-IR	quartz	MCT-A [‡]	11,700 - 2,800*	ETC, white light
		MCT-B [‡]	11,700 - 2,800*	ETC, white light

continued...

Light Range	Beamsplitter	Detector	Spectral Range (cm ⁻¹)	Source	
Near-IR, <i>continued</i>	CaF ₂	InSb ^{†,§}	11,500 - 2,800*	ETC, white light	
		PbSe	13,000 - 2,800*	ETC, white light	
		PbS TEC (with SabIR™)	10,000 - 4,200*	ETC, white light	
		InGaAs	12,000 - 3,800	ETC, white light	
		MCT-A [‡]	11,700 - 1,200*	ETC, white light	
		MCT-B [‡]	11,700 - 1,200*	ETC, white light	
		InSb ^{†,§}	11,500 - 1,850*	ETC, white light	
		PbSe	13,000 - 2,000*	ETC, white light	
		PbS TEC (with SabIR)	10,000 - 4,200*	ETC, white light	
		InGaAs	12,000 - 3,800	ETC, white light	
		XT-KBr	MCT-A [‡]	11,000 - 600*	ETC, white light
			MCT-B [‡]	11,000 - 400*	ETC, white light
			InSb ^{†,§}	11,000 - 1,850*	ETC, white light
			PbSe	11,000 - 2,000*	ETC, white light
			DLaTGS-KBr	11,000 - 375*	ETC, white light
			DLaTGS TEC	11,000 - 375*	ETC, white light
			InGaAs	12,000 - 3,800	ETC, white light
			mid-IR	KBr	DLaTGS-KBr
MCT-A [‡]	7,400 - 600	ETC			
MCT-B [‡]	7,400 - 400	ETC			
DLaTGS TEC	7,100 - 350	ETC			
DLaTGS-Csl	6,400 - 350	ETC			

continued...

Light Range	Beamsplitter	Detector	Spectral Range (cm ⁻¹)	Source
Mid-IR, <i>continued</i>	CsI [♣]	DLaTGS-CsI	6,400 - 225	ETC
		MCT-A [‡]	6,400 - 600	ETC
		MCT-B [‡]	6,400 - 400	ETC
	ZnSe	DLaTGS-KBr	4,000 - 650	ETC
		MCT-A [‡]	4,000 - 650	ETC
		MCT-B [‡]	4,000 - 650	ETC
		DLaTGS TEC	4,000 - 650	ETC
far-IR	Solid-Substrate [™]	DLaTGS-CsI	4,000 - 650	ETC
		DLaTGS-PE	700 - 50	ETC
		Si bolometer	700 - 20	ETC

Notes:

- * This spectral range reflects the combination of the ranges of the ETC and white light sources, the limits of the beamsplitter-detector combination, and the aluminum optics. The range achieved using one of these sources will not be as broad as the total range shown.
- † Si detectors can be used only with a white light (tungsten-halogen) source.
- ‡ These detectors must be cooled with liquid nitrogen before use.
- § InSb detectors will not produce a signal under intense light. During installation and alignment, start with the smallest aperture setting.
- ♣ CsI beamsplitters are extremely hygroscopic (sensitive to moisture).



In SST Help Topics view “Detector specifications” for more detailed detector specification information.

Improving the quality of your spectral data

If you are using the spectrometer for quantitative analysis or other demanding applications, you are concerned with the precision and accuracy of your spectra. For these types of applications it is important that the spectra you collect have high wavelength precision. This means that the frequency axis (X-axis) location of peaks in a spectrum is consistently reproducible and within IUPAC (International Union of Pure and Applied Chemistry) published specifications. You must also be certain that your spectrometer responds linearly to the samples you are studying. This means that absorption band intensity is directly proportional to the number of molecules subjected to the light beam; thus, as the number of molecules in the beam increases, the detected absorbance signal also increases at a consistent rate.

If you are studying samples that produce tiny spectral peaks or have weak spectral features, or if you are looking for small changes in your samples, make sure the signal-to-noise ratio is high enough to let you distinguish spectral features from the noise inherent in all experimental data. This prevents the signals containing spectral information from being lost among the signals generated by the random movement of electrons, building vibrations, light source fluctuations and other such sources.

Improving linearity and photometric accuracy

Some detectors (including PbSe, Si, MCT-A and InSb detectors) are highly sensitive and can become saturated or produce a distorted (non-linear and photometrically inaccurate) signal if the light energy is not reduced before it reaches the detector element or if the detector gain is set too high.

Look at a single-beam spectrum in the low-end region around 600 to 375 cm^{-1} . You should see a straight line very near 0 intensity units. As a rule of thumb, the distance from 0 to the baseline should be less than 1% of the spectrum's maximum intensity value.

If the detector is saturated, you will see false energy in the low-end region. The baseline might be far above zero. If the distance from the baseline to 0 is greater than 20% of the spectrum's maximum intensity value, your detector electronics may be overloaded. Contact technical support for assistance.

Note The maximum intensity of a mid-IR single-beam spectrum is typically found near $2,000\text{ cm}^{-1}$. ▲

The distorted signal may cause problems with photometric accuracy. For good quantitative data, the sample and background interferograms should be about the same size. Scattering samples and very dense samples produce very small signals that, when compared with much larger background signals, can distort quantitative data. Check the background and sample interferograms. If you see a substantial difference in their sizes, photometric accuracy could be a problem.

To solve these problems, use one the following to modify the infrared beam:

- Use a bandwidth-limiting filter.
- Use an energy screen.
- Adjust the aperture setting.



In Spectrometer Help Topics view “Setting up experiments” for instructions for using filters and energy screens.

When to use filters

Use bandwidth-limiting filters to improve the signal-to-noise ratio of the data and also prevent detector saturation by allowing only energy in your particular area of interest to pass to the detector element.

An optional filter wheel lets you automatically move a filter into the beam path before collecting data. See “Using the filter wheel” in the “Spectrometer Options” chapter for more information.



In Spectrometer Help Topics view “Setting up experiments” for instructions for installing filters in the sample compartment or optional filter wheel.

When to use energy screens

Depending on the types of detectors you use, your system may include a set of four energy screens. These metal screens help prevent detector saturation and signal distortion by blocking out a portion of the energy at all frequencies of the infrared beam. If your experiments deal with information from a broad range of frequencies, these screens may be the most effective means of reducing the light level.

The energy screens are labeled A, B, C and D. The following table shows the percentage of the infrared energy that each screen passes. It also lists the detectors typically used with each screen, as a starting point for correcting linearity problems.

Screen	% Transmitted*	Detectors Typically Used With Screen
None	100	DLaTGS
A	30	MCT-A
B	10	
C	3	
D	1	

* These are nominal values that may vary due to diffraction and detector variations.

To correct for photometric accuracy, you may need to add a “heavier” screen (one that transmits less infrared energy). With corrections for photometric accuracy you will notice some reduction in the signal-to-noise ratio but will obtain more reliable quantitative data. Generally, the signal-to-noise ratio reduction is less than the signal intensity.



In Spectrometer Help Topics view “Setting up experiments” for instructions for installing energy screens in the sample compartment.

An optional energy screen wheel lets you automatically move a screen into the beam path before collecting data. See “Using the energy screen wheel” in the “Spectrometer Options” chapter for more information.

When to change the aperture setting

The aperture in a Nicolet 8700 is a variable-diameter opening that controls the angular size of the infrared beam and, thus, the amount of radiation that reaches the sample. Using the aperture has these advantages:

- It lets you use more sensitive detectors.
- It helps prevent infrared energy saturation, so the response of the detector is more linear.
- It improves wavenumber accuracy and resolution by acting as a point source of infrared radiation.

In general you will find that the larger the aperture, the better is the signal-to-noise ratio of the collected data. The smaller the aperture, the better the stability and accuracy will be. Small apertures are needed for high-resolution experiments.

DLaTGS detectors can accommodate most of the energy from the source, which means you should use a large aperture size. Detectors that require cooling with liquid nitrogen are very sensitive and require a small aperture size or the use of an energy screen (see the preceding section for more information).

Note Aperture parameter setting determines the *area* of the aperture opening. The light energy is proportional to the aperture area. A setting of 100 gives a nominal aperture diameter of 8 mm and an approximate area of 0.50 cm². ▲

The following table lists recommended aperture settings for different detectors with the appropriate energy screen installed. (See the preceding section for information about the correct energy screen to use for each detector type.) The settings in the table are based on the physical size of the detector elements and maximize the amount of infrared energy that reaches the sample. To correct linearity and photometric accuracy problems, you can reduce the setting, but you will pay a price in terms of the signal-to-noise ratio.

Detector	Aperture Setting
DLaTGS	100
MCT-A, MCT-B, InSb, PbSe, Si, InGaAs	32



In OMNIC Help Topics find “aperture” in the Index and go to “Setting the aperture size” for information about changing the aperture setting.

How to improve the signal-to-noise ratio

If you primarily analyze qualitative data, you may wish to optimize the system for a better signal-to-noise ratio. This can be particularly important when you are working with scattering samples and samples that absorb more infrared energy. These samples produce smaller signals that can be “lost” in the noise.

There are several ways to improve the signal-to-noise ratio. The most commonly used method is to increase the number of scans. This both reduces the noise level and makes small absorptions easier to distinguish. You can also improve the ratio by reducing the resolution (that is, using a higher Resolution setting).

Another method is to use an energy screen that transmits more light (or no screen at all). In this case, the resulting spectrum might be distorted and accuracy and stability could be reduced. Checking the single-beam baseline in the region below the low-end cutoff will give you a rough idea of how much distortion is occurring. If the distance from the baseline to 0 is more than 15% of the spectrum's maximum intensity value, you may have difficulty reproducing the results.

Note If the distance from the baseline to 0 is greater than 20% of the spectrum's maximum intensity value, your detector electronics may be overloaded. Contact technical support for assistance. ▲



In Spectrometer Help Topics view “Setting up experiments” for instructions for installing filters and energy screens.

How to improve resolution

If you want to achieve higher resolution, you may need to use a smaller aperture setting and an energy screen that transmits more light (or no screen at all). Your spectroscopy software will automatically change the aperture setting if a smaller beam size is required. Be aware that the smaller beam size will reduce the signal-to-noise ratio.



In OMNIC Help Topics find “aperture” in the Index and go to “Setting the aperture size” for information about changing the aperture setting.

Choosing the right moving mirror velocity

While a wide range of moving mirror velocities are available on Nicolet 8700 spectrometers, some velocity settings cannot be used for collecting data at certain combinations of spectral range and resolution:

If you are collecting data over a spectral range above 7899 cm^{-1} , optical velocity settings faster than 2.53 cm/s are not available.

To specify the optical velocity and spectral range, set Velocity and Spectral Range on the Bench tab of the Experiment Setup dialog box. To specify the resolution, set Resolution on the Collect tab.

Notice When you switch to a different detector or beamsplitter, OMNIC automatically resets the default spectral range in the Experiment Setup dialog box. Be sure to check the range and set the velocity to a value that is appropriate. ▲

Choosing the right scan velocity

To allow you to collect data faster, OMNIC SST and your Nicolet 8700 spectrometer support increased linear scan velocities, up to 8.2277 cm/s. These higher velocities are useful for experiments where the sample is likely to change over time. The highest of these velocities will be used when you perform rapid-scan experiments using OMNIC Series.

While a wide range of optical velocities (optical velocity is twice the mirror velocity) are available on the Nicolet 8700, some velocity settings cannot be used for collecting data at certain combinations of spectral range and resolution. The following tables show which velocity settings (in cm/s) are available for different resolution settings (in wavenumbers) under the specified conditions. A check mark (✓) indicates that the setting is available; a dash (—) indicates that the setting is not available.

When sample spacing is set to 4 or 2 or the upper limit of the spectral range is less than or equal to 7,899 wavenumber:

Resolution →	0.125	0.25	0.5	1.0	2.0	4.0	8.0	16.0	32.0
Optical Velocity ↓									
0.0158 - 5.6961	✓	✓	✓	✓	✓	✓	✓	✓	✓
6.3290	—	—	✓	✓	✓	✓	✓	✓	✓
6.9619	—	—	—	—	✓	✓	✓	✓	✓
7.5948	—	—	✓	✓	✓	✓	✓	✓	✓
8.8617	—	—	—	—	—	✓	✓	✓	✓

When sample spacing is set to 1 or the upper limit of the spectral range is within the 7900 to 15798 wavenumber range:

Resolution →	0.125	0.25	0.5	1.0	2.0	4.0	8.0	16.0	32.0
Optical Velocity ↓									
0.0158 - 2.5317	✓	✓	✓	✓	✓	✓	✓	✓	✓
3.1647 - 3.7974	—	—	—	✓	✓	✓	✓	✓	✓
4.4303	—	—	—	—	—	—	✓	✓	✓
4.7468 - 5.6961	—	—	—	—	—	—	—	✓	✓
6.3290	—	—	—	—	—	—	—	—	✓
6.9619 - 8.8617	—	—	—	—	—	—	—	—	—

When sample spacing is set to 0.5 or the upper limit of the spectral range is within the 15799 to 31596 wavenumber range:

Resolution →	0.125	0.25	0.5	1.0	2.0	4.0	8.0	16.0	32.0
Optical Velocity ↓									
0.0158 - 1.2659	✓	✓	✓	✓	✓	✓	✓	✓	✓
1.8988	—	—	—	—	—	✓	✓	✓	✓
2.5317	—	—	—	—	—	—	—	—	✓
3.1647 - 8.8617	—	—	—	—	—	—	—	—	—

To specify the optical velocity and spectral range, set Velocity and Spectral Range on the Bench tab of the Experiment Setup dialog box. To specify the resolution, set Resolution on the Bench tab.

- Notice** When you switch to a different detector or beamsplitter, OMNIC automatically resets the default spectral range in the Experiment Setup dialog box. Be sure to check the range and set the velocity to a value that is appropriate (see the limitations described above). ▲
- Note** When collecting rapid scan data with a sampling interval of less than 0.04 second, do not interact with the computer (with the mouse or keyboard) until the collection is finished; otherwise, Windows may interrupt the collection. The current sampling interval is shown on the Collect tab of the Series Setup dialog box and is calculated from the resolution, mirror velocity and number of scans per spectrum or interferogram. ▲

How to collect slow-scan data

Slow scan allows the moving mirror to be precisely controlled at very low velocities. Among other applications, this is particularly useful for photoacoustic experiments. Slow scan is an experimental technique and we invite you to explore new applications.

As with other linear applications, data in slow-scan applications is collected continuously, as the moving mirror travels at a constant velocity within the interferometer. Each light wave is modulated individually, with the modulation frequency equal to the mirror velocity multiplied by the wavelength of the light wave.

Due to the low velocities, you will notice a decrease in the signal-to-noise ratio in slow-scan experiments. You can improve it by increasing the number of scans.

No special hardware setup is required for slow-scan experiments. Nearly any hardware you use for other linear scan experiments can be used for slow-scan experiments. Some experiments that are usually run in step-scan mode (such as photoacoustic spectroscopy) can also be run using slow-scan.

Note Reduce the aperture setting or use an appropriate filter or screen when running slow-scan experiments to prevent saturating the DLaTGS, photoacoustic or other thermal detector. If you are not using a filter or energy screen, an aperture setting of 2 is common for slow-scan experiments. ▲

A note about vibrations

While any application can be effected by vibrations, slow-scan experiments are prone to disruption from vibrations. Should your experiment be disrupted, the Nicolet 8700 spectrometer will automatically recover. You do not need to restart the data collection.

If your experiment is disrupted by vibration, you can expect to hear a clicking sound as the moving mirror is repositioned. This may take a minute or two. Once the mirror is repositioned, data collection will resume from the last valid scan.

Running slow-scan experiments

The slow-scan capabilities are available on the Bench tab of the Experiment Setup dialog box.

Use the Velocity setting on the Bench tab to access slow scan. Selecting any of the velocities below 0.1581 cm/s puts the spectrometer in slow-scan mode. Use Collect Sample and Collect Background in the Collect menu to start your slow-scan experiments.

How to collect data in the visible spectral range

The ability of the spectrometer to collect data is affected by the detector-beamsplitter combination and any energy screens or optical filters that are installed in the spectrometer. For example, if you use an optional quartz beamsplitter, a silicon detector and a white-light source, the sampling range is extended to 27,000 cm^{-1} .

Since silicon detectors are very sensitive, you will also need to install an energy screen or bandwidth-limiting filter to prevent the detector from being saturated during the experiment. The following table lists a variety of spectral bands in the extended spectral range and lists the filter or energy screen that should be used to obtain data in each range. It also lists typical aperture and gain settings for experiments in each range.

Spectral Range	Filter or Screen	Aperture	Gain
16,000 - 9,000 cm^{-1}	red filter	32	1
16,000 - 9,000 cm^{-1}	energy screen A	32	1
23,000 - 16,000 cm^{-1}	broad-band blue filter	100	8
26,000 - 21,000 cm^{-1}	narrow-band blue filter	100	8

You can use these filters and settings as a starting point and vary them as required by your experimental conditions. To set the aperture and gain, set the Aperture and Gain parameters on the Bench tab in the Experiment Setup dialog box.



In Spectrometer Help Topics view “Setting up experiments” for instructions for installing filters and energy screens.

The optional filter wheel and energy screen wheel let you automatically move a filter and energy screen into the beam path before collecting data. See “Using the filter wheel” and “Using the energy screen wheel” in the “Spectrometer Options” chapter for more information.

How to collect data in the extended spectral range

With OMNIC SST, the true spectral sampling range of your spectrometer has been extended to $31,596\text{ cm}^{-1}$. You can make use of this range by setting Sample Spacing on the Advanced tab of the Experiment Setup dialog box to 0.5 whenever you specify a spectral range (on the Bench tab of the Experiment Setup dialog box) that exceeds $15,798\text{ cm}^{-1}$. When you use a sample spacing of one-half, four data points are collected during one laser period. (A setting of 1 collects data twice, a setting of 2 collects data once, and a setting of 4 collects data once for every two laser periods.)

Using a *higher* setting of Sample Spacing results in *fewer* collected data points, which allows you to use a *faster* scan velocity. With this increase in velocity, *less* time is required for data collection. In step-scan experiments, the sample spacing setting alone can be used to shorten collection time.

There are some constraints on using sample spacing to shorten data collection time and still collect valid data. For example, the Sample Spacing parameter determines the nominal free (also known as nonaliased or nonambiguous) spectral range that you can reliably study, due to the Nyquist, or Sampling, theorem. The Nyquist theorem states that at least two data points must be collected per period if you wish to reproduce the waveform accurately from discrete sampling.

Since a 15798 cm^{-1} frequency laser is used to trigger data collection, sample spacing limits the free spectral range for your interferogram as follows.

Sample Spacing	Nominal Free Spectral Range
0.5	31,596 to 0 cm^{-1}
1	15,798 to 0 cm^{-1}
2	7,899 to 0 cm^{-1}
4	3,949 to 0 cm^{-1}

If you allow energy from outside the free spectral range to reach the detector, you will find that it corrupts your data with false energy. To prevent this corruption, use an optical filter to prevent the unwanted energy from reaching the detector and use an appropriate beamsplitter-detector combination.

As an example, OMNIC uses a sample spacing of 2 for all experiments where the data is collected in the region below 7899 cm^{-1} . You can run these experiments using the standard DLaTGS/KBr detector-beamsplitter combination, since this combination passes no energy above 7899 cm^{-1} . No additional optical filters are required in this case.

However, if you are studying only data below 3940 cm^{-1} , you can use the sample spacing setting (along with the Velocity parameter) to cut the data collection time in half with little or no effect on the signal-to-noise ratio. For these experiments you would set Sample Spacing to 4 and prevent energy above 3940 cm^{-1} from reaching the detector.



In OMNIC Help Topics find “sample spacing” in the Index and go to “Specifying the sample spacing” for more information about Sample Spacing.

There are several ways to prevent unwanted energy from reaching the detector. The most common is to install a 3940 cm^{-1} low-pass optical filter in the beam path.



In Spectrometer Help Topics view “Installing an optical filter” in the “Setting up experiments” book for instructions on installing filters.

As an alternative, you could install a band-pass filter (centered around your particular region of interest). If you choose a band-pass filter for use with a sample spacing of 4, make sure the upper limit of the filter is 3940 cm^{-1} or lower. No filtering would be required for experiments that pass no energy above 3940 cm^{-1} to the detector.

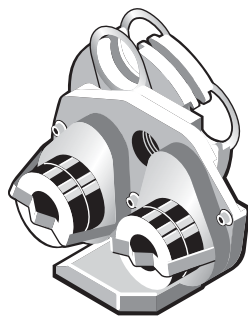
Spectrometer Options

This chapter explains how to use these optional spectrometer features:

- The **automated filter wheel** moves optical filters (supplied by you) into the beam path.
- The **energy screen wheel** moves an energy screen into the beam path to reduce the energy reaching the detector.
- The **polarizer** allows you to control the orientation of the electric field vector of the infrared beam entering the sample compartment.
- The **detector interface** allows OMNIC to recognize and control external detectors that were not made by Thermo Fisher.

Using a filter wheel

The optional filter wheel accessory lets you automatically insert optical filters (band-pass, low-pass or high-pass) into the beam path. This lets you reduce the amount infrared light that reaches the detector in a spectrally selective way. This is particularly useful for studies of small spectral regions or for blocking noisy spectral regions that contain no data of interest. Energy from other regions does not reach the detector, thus improving the signal-to-noise ratio in the region of interest.

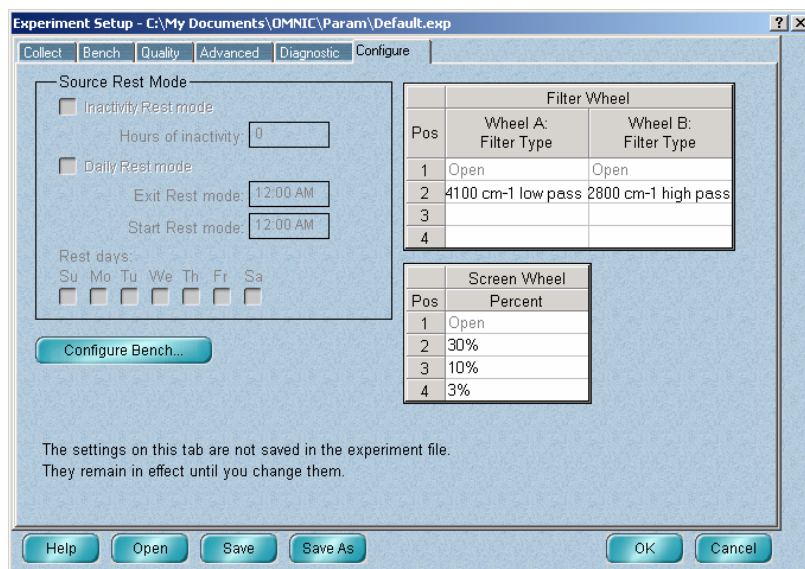


The accessory has two wheels: wheel A is closer to the source. Each wheel can be moved to one of four positions. Both wheel A and wheel B have an open position for collecting spectra without a filter in the beam path. Positions 1, 2 and 3 are available for filters that you provide. Each position accepts one 1 mm thick or one 4 mm thick filter that is 1-inch in diameter. Spacers are provided to secure 1-mm filters in position.



In Spectrometer Help Topics view “Installing an optical filter in the automated filter wheel” in the “Setting up experiments” book for instructions for installing filters in the wheel.

Once you have installed your filters, enter their descriptions into OMNIC using the Filter Wheel table on the Configure tab of the Experiment Setup dialog box. Be descriptive.

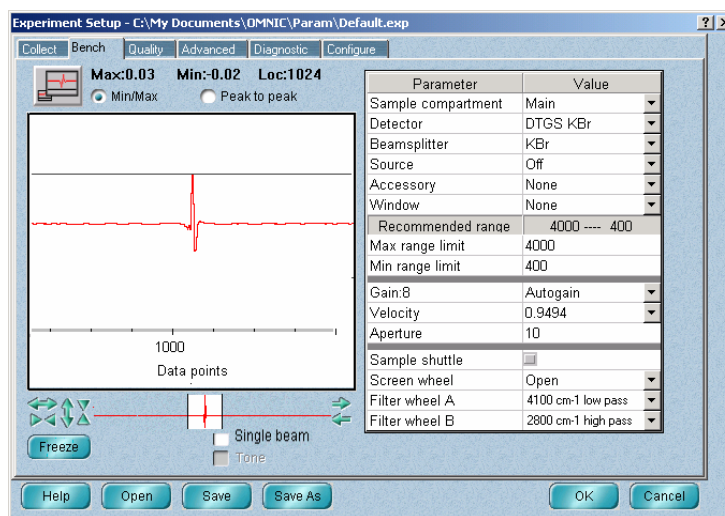


In OMNIC Help Topics find “filter wheel” in the Index and go to “Entering descriptions of the filters in the filter wheel” for more detailed instructions.

Your filter descriptions will be saved in the experiment file and are available for selection through the Filter Wheel A and Filter Wheel B parameters on the Bench tab of Experiment Setup. Your descriptions of the filters used during data collection also are saved in the collection and processing information for the spectra you collect.

By controlling which position of each wheel is in the beam path, you can collect spectra with no filter, just one filter or a combination of two filters. For example, you could install and select a band-pass filter to block out frequencies in both the high and low ends of the spectral range, resulting in a spectrum with absorptions only in the middle of the range. You also could accomplish mid-range data collection using a high-pass filter installed in one wheel and a low-pass filter installed in the other.

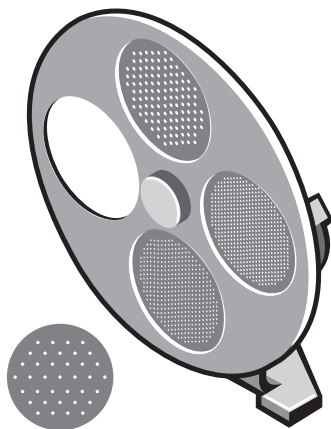
To specify the filter(s) to use for an experiment, set Filter Wheel A and Filter Wheel B on the Bench tab of the Experiment Setup dialog box (available through Experiment Setup in the Collect menu).



In OMNIC Help Topics find “filter wheel” in the Index and go to “Controlling the filter wheel” for more detailed instructions.

Using an energy screen wheel

The optional energy screen wheel lets you automatically insert an energy screen into the beam path to block out a portion of the energy at all frequencies of the infrared beam. This is useful for preventing detector saturation and signal distortion. For more information about using energy screens, see “When to use energy screens” in the “Spectrometer Basics” chapter.

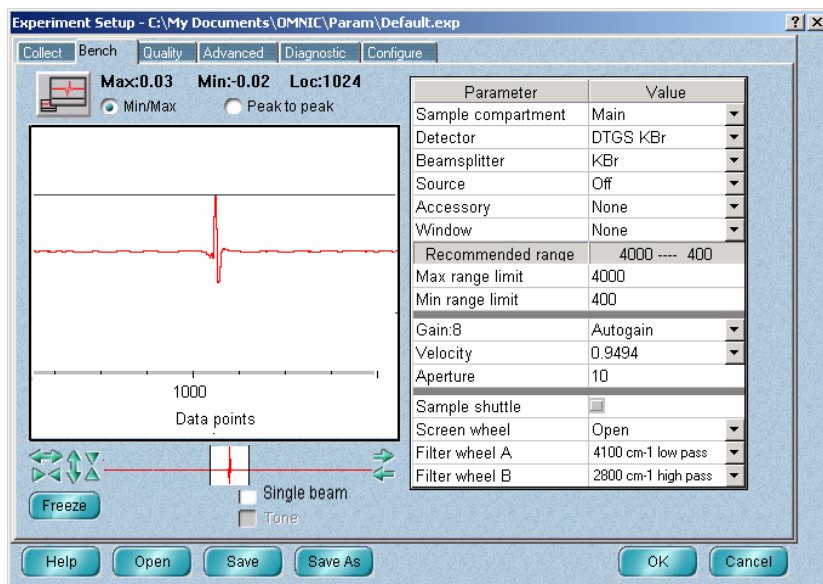


The wheel can be moved to any of four positions: an open position (for collecting spectra without a screen in the beam path) and 3 screen positions. As shipped from the factory, the screen positions are populated with 30%, 10%, and 3% screens. The Screen Wheel parameters in Experiment Setup to describe the percentage of light transmitted by each screen installed in the wheel. Simply select one to move the screen into the beam path.

To specify the screen to use for an experiment, set Screen Wheel on the Bench tab of the Experiment Setup dialog box (available through Experiment Setup in the Collect menu).



In OMNIC Help Topics find “energy screen wheel” in the Index and go to “Controlling the energy screen wheel” for complete instructions.

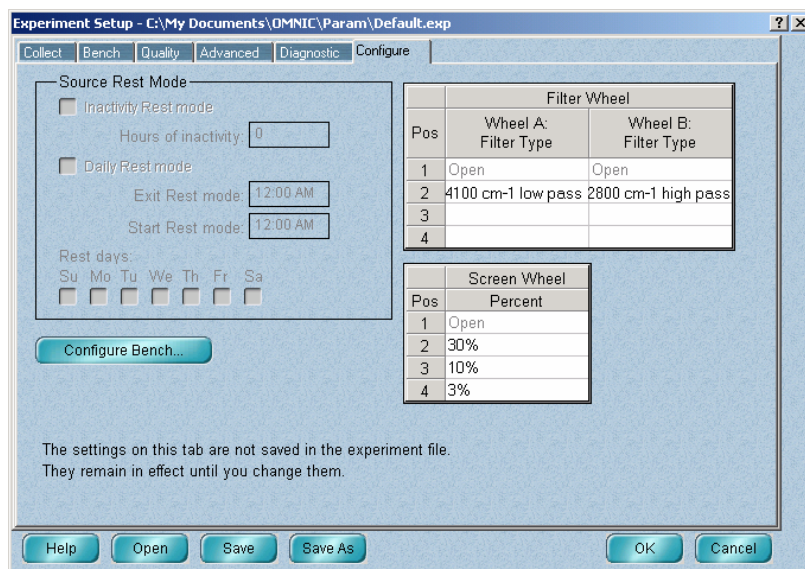


After you have moved a screen into the beam path, you can see its effect on the signal intensity in the live display on the Bench tab. This helps you select the optimum screen for a particular sample.

A 1% screen also is shipped with the wheel. Contact technical support if you wish to use this or other screens that you provide in the wheel. If you use the 1% screen or one of your own, be sure to change the description of the screen position on the Configure tab.



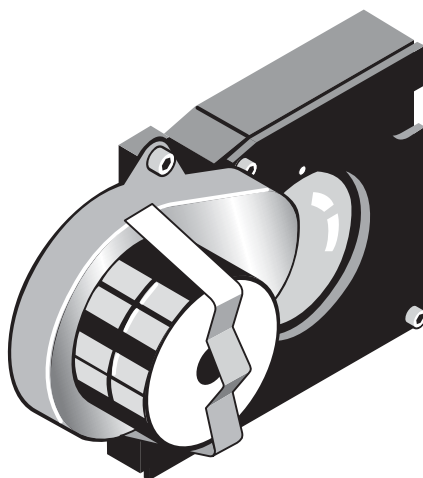
In OMNIC Help Topics find “energy screen wheel” in the Index and go to “Specifying the energy screens in the energy screen wheel” for more detailed instructions.



If you have OMNIC Series, you can display the series of spectra collected in this way. To create a series (.SRS) file from your spectra, follow the instructions in “Creating a series data set” in the “Series Menu Commands” chapter of the OMNIC Series User's Guide.

Using an internal polarizer

An optional automated polarizer lets you automatically control the orientation of the electric field vector of the IR beam entering the sample compartment. The range of orientation is 0 to 180 degrees in increments of 1 degree. At 0 degrees, the electric field vector is oriented vertically, perpendicular to the sample compartment base plate. This option is useful for performing polarization studies of thin films and other sample types.



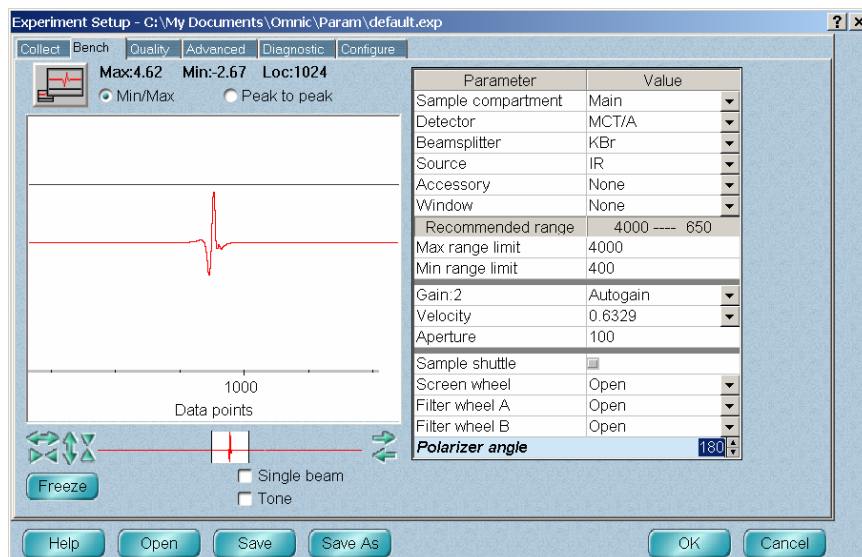
Note The polarizer cannot be installed on spectrometers with sample compartment windows. ▲



In Spectrometer Help Topics view “Installing optional hardware” for detailed information about installing the polarizer.

In these experiments, a unique background is required for each polarization position used. For example, if you are going to collect spectra at 0 and 90 degrees, corresponding background spectra are required at 0 and 90 degrees.

To set the polarization angle, type any number from 0 to 180 in the Polarizer Angle text box on the Bench tab of the Experiment Setup dialog box (available through Experiment Setup in the Collect menu). Use the up and down arrows to step the polarizer one degree at a time to optimize your signal.



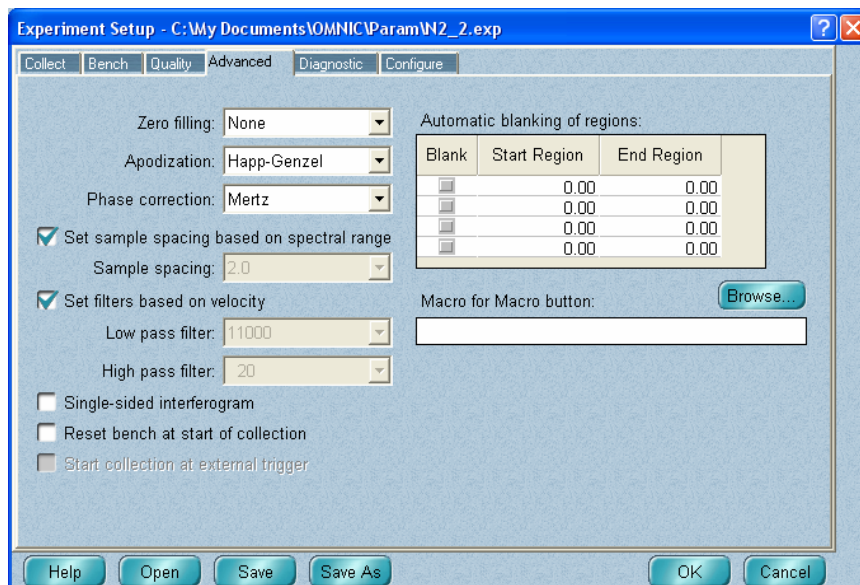
In OMNIC Help Topics find “polarizer” in the Index and go to “Controlling the polarizer” for more detailed instructions.

Begin your experiment by collecting backgrounds (as single beam spectra) at each polarizer angle required by your experiment. Save each background spectrum with a unique, descriptive name, such as Background 0, Background 90. Once the background spectra are collected and saved, you can begin to collect sample spectra. Sample data may be collected and saved as single beam spectra. Once data collection is complete, use the appropriate background file to reprocess the data into your final format. Sample data also may be collected and saved as ratioed spectra (%T, A, %R etc.) using the corresponding stored background. Use the Background Handling parameter on the Collect tab in Experiment Setup to specify the background file name. Click the Use Specified Background File checkbox and then enter the background spectrum filename.

If you have OMNIC Macros\Basic or OMNIC Macros\Pro, you can create a macro that changes the angle incrementally with each successive set of background and sample spectra.



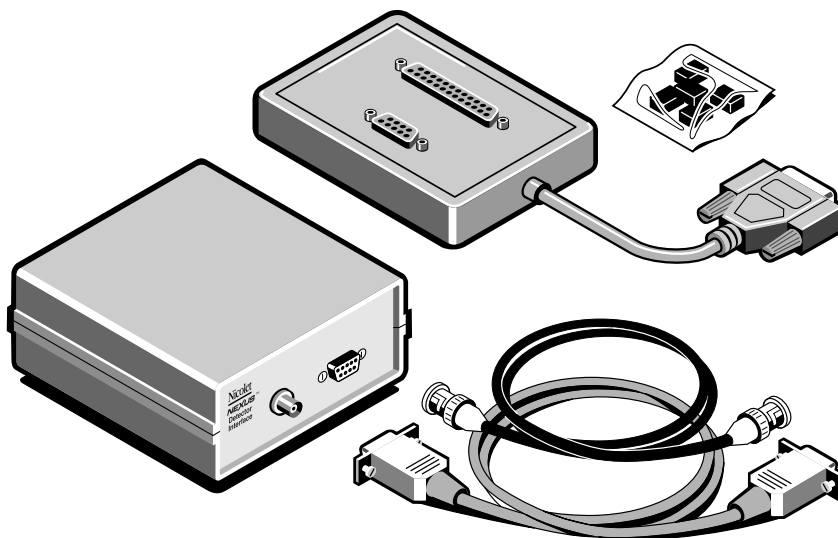
Then use Experiment Setup to specify that the Macro button start the experiment and run the macro. Use the Macro for Macro button field on the Advanced tab in Experiment Setup dialog box (available through Experiment Setup in the Collect menu) to specify the macro to run. You may browse to locate the macro file or type the full path and file name into the text field.



If you have OMNIC Series, you can display the series of spectra collected in this way. To create a series (.SRS) file from your spectra, follow the instructions in “Creating a series data set” in the “Series Menu Commands” chapter of the OMNIC Series User's Guide.

Using a detector interface kit

A variety of accessories contain detectors that are automatically recognized by Nicolet, Nexus™ and Magna-IR™ spectrometers. The detector interface accessory allows other external detectors to be recognized.



Before you connect the detector interface to your detector or your spectrometer, you must configure it for an unused detector address and the appropriate detector type. Once the interface is configured and connected, you can use Experiment Setup to select the detector for use in your experiments.



In SST Help Topics, see “Detector interface” in “Hardware setup > Optional kits” for detailed instructions about configuring and connecting the interface kit.

Accessories

This chapter briefly describes the types of sampling and system accessories that are available for your spectrometer. Complete descriptions and operating instructions are included with the accessories.

Smart Accessories

In addition to traditional accessories, a variety of Smart Accessories are available for your spectrometer. Nicolet FT-IR spectrometers identify each Smart Accessory as it is installed and set the software parameters for data collection. Also, a series of spectral quality checks are performed to ensure that the accessory is installed and operating correctly.



Detailed tutorials for installing, operating and maintaining each Smart Accessory are provided on-line. To start a Smart Accessory tutorial, click Sampling Techniques in the Help menu and then click the accessory name.

Smart ARK™ – This is a horizontal ATR (attenuated total reflection) accessory with high stability, complete purge capabilities, tool-free alignment and high performance specifications. It includes integral purge tubes that seal the accessory from the atmosphere, and a cast aluminum body for exceptional stability.

Smart Collector™ – Diffuse reflection enables analysis of highly light-scattering solids that are difficult to analyze using transmission techniques. This method is also useful when the sample, usually a powder, must be analyzed without modification.

Smart Diffuse Reflectance – The diffuse reflection technique lets you analyze highly light-scattering solids that are difficult to analyze using transmission techniques. The technique is also useful when the sample, usually a powder, must be analyzed without modification. This accessory lets you analyze a wide variety of sample types and features integral sample cups for convenient, fast sampling.

Smart DuraSamplIR™ – This single-reflection horizontal ATR accessory has a viewing feature that makes it easy to position the sample and monitor the applied pressure. The accessory is ideal for small samples and can be used to measure liquids, powders and pliable solids

Smart DuraScope™ – The Smart DuraScope combines the benefits of a diamond ATR element with video enhancement to create an analysis tool for a wide range of sample types, from large, hard materials to small inclusions and contaminants. You can position the sample while looking through the diamond ATR element. This helps you manipulate micro samples to achieve optimum contact with the crystal, resulting in superior quality spectral data.

Smart Endurance™ – This single-reflection diamond ATR accessory is rugged and versatile. It stands up to highly corrosive, caustic, intractable or abrasive samples, making it a good choice for almost any sample type.

Smart Golden Gate™ – This is a horizontal, single-reflection ATR accessory that features an extremely durable diamond crystal. It handles a wide range of sample types, including hard or brittle solids, corrosive liquids and hard **powders**.

Smart Integrating Sphere – The Smart Integrating Sphere is a highly efficient collector of diffuse scattered radiation. Light enters the integrating sphere from the bottom. The light then strikes the sample and is diffusely reflected. The reflected light is collected by the sphere and directed onto the detector. The optional sample spinner allows a wide area from inhomogeneous materials, like pellets or powders, to be analyzed

Smart Mid-IR FiberPort – This high-throughput accessory lets you analyze liquids remotely. The needle probe can reach “hard to get” samples, such as liquids in micro containers, hazardous environments or remote locations. The FiberPort is a unique optical interface that transfers IR energy from the spectrometer to the fiber optic cables and probes. A complete line of fiber optic probes is available for sampling a wide range of sample types.

Smart MIRacle™ – This is a single-reflection horizontal ATR accessory with exceptional throughput and sensitivity. It can use several crystal types and has a micrometer screw for precise control of applied pressure.

Smart Multi-Bounce HATR – This multi-reflection horizontal ATR accessory has a shorter pathlength and higher throughput than traditional HATR accessory designs. It is the best choice for routine analysis of strong infrared-absorbing samples. This accessory is ideal for rapid quantitative and qualitative analyses, since sample preparation is usually not necessary.

Smart OMNI-Sampler™ – This single-reflection ATR accessory features a spherical crystal that lets you measure a wide variety of sample types. The unique tower design automatically applies the optimum pressure while protecting the crystal. The accessory is ideal for analyzing very small samples or sample areas and provides high reproducibility.

Smart OMNI-Transmission™ – This easy-to-install transmission accessory lets you sample liquids, gases and solids using a wide variety of transmission cells and infrared cards.

Smart Orbit™ – This single-reflection ATR accessory features a durable diamond crystal and a swivel pressure tower that ensures consistent pressure from sample to sample. You can use the accessory to perform analyses from the near-IR to the far-IR.

Smart Performer™ – This single-reflection ATR accessory features a horizontal sampling surface for collecting high quality spectra with minimal sample preparation. The accessory uses a wide variety of low cost crystals that are easy to install and remove.

Smart Refractor™ – This top-loading accessory is designed for fast analysis of coatings on reflective substrates using the grazing angle specular reflection technique.

Smart SAGA™ – This advanced accessory is designed for the analysis of thin films on reflective substrates. The 80 degree angle of incidence for this reflection-absorption accessory allows sensitive measurements of films as thin as 0.1 nm.

Smart SpeculATR™ – This single-bounce horizontal ATR/specular reflection accessory allows versatility in measurement where a range of sample morphologies may need to be analyzed.

Smart SplitPea™ – This horizontal ATR microsampling accessory is designed for fast analysis of solids, liquids, and powders. It is ideal for analyzing hard materials, small samples or samples where only minute quantities are available.



In OMNIC Help Topics find “accessory” in the Index and go to “Specifying the accessory” for instructions for setting up and saving experiments for custom accessories.

Other sampling accessories

You can install many of the sampling accessories yourself. After you install an accessory, you may have to align it. Instructions for aligning the spectrometer are included in the “Maintenance and Service” chapter of this manual. Instructions for aligning an accessory are provided in the documentation that came with that accessory.



Some accessories fit into the sample compartment and require that you remove the Snap-In baseplate before installing the accessory. For information about using Snap-In baseplates, view “Removing the Snap-In baseplate” in the “Setting up experiments” book in Spectrometer Help Topics.

Note

Additional Snap-In sample compartment baseplates are available for use with each accessory to make changing accessories easier. ▲

Call Thermo Fisher if you are interested in ordering any of the following sampling accessories.

Absolute transmission accessory – This accessory allows for the measurement of absolute transmission of samples with reflective surfaces. The design prevents energy reflected from the sample from entering the interferometer for remodulation. Using this accessory involves replacing pinned-in-place mirrors before and after the sample compartment.



For information about installing an absolute transmission accessory, view “Replacing the parabolic mirror” in the “Setting up experiments” book in Spectrometer Help Topics.

Automatic sample wheel – This accessory holds multiple samples and rotates them into the beam path for data collection. The sample wheel is commonly used to measure multiple polymer or pressed-powder samples automatically.

Auxiliary experiment module (AEM) – The AEM provides you with an additional sample compartment. You can position it on the right or left side of the spectrometer. With an AEM installed, you can run routine analyses with the spectrometer and quickly switch beam paths to the AEM to collect data from other samples without removing accessories from the main sample compartment. Any accessory or detector that can be installed in the spectrometer can be installed in the AEM. The AEM has two detector locations.

Centaurus™ and Continuum™ infrared microscopes – Thermo Fisher offers microscopes that attach directly to the side of the spectrometer. Microscopes can be installed between the spectrometer and other accessory modules. The microscopes provide fast, nondestructive microanalysis with minimal sample preparation and alignment.

Custom accessory baseplate – You can use this Smart baseplate to mount an accessory you have built or purchased from another manufacturer. When you install the accessory and baseplate in the sample compartment, the system automatically selects the Custom Accessory experiment (or allows you to select from the experiments you have saved for the baseplate).

Detector interface kit – A variety of accessories (that were specifically designed for Nicolet 8700 spectrometers) contain detectors that are automatically recognized by your spectrometer. The detector interface accessory allows your spectrometer and OMNIC software to recognize other detectors, including non-Nicolet detectors.



For information about installing and using a detector interface kit, view “Detector interface” in the “Optional kits” book in OMNIC SST Help Topics.

Energy screen wheel – This accessory lets you prevent detector saturation and signal distortion by using a screen to block a portion of the infrared energy. See “Using the energy screen wheel” in the “Spectrometer Options” chapter for complete information.

Filter wheel – This accessory lets you control the spectral range of the infrared light that reaches the detector by inserting low pass or high pass filter into the beam path. See “Using the filter wheel” in the “Spectrometer Options” chapter for complete information.

Foundation Series – The innovative modular design of this accessory family provides access to several sampling devices using a common base. This allows experimental flexibility and an economical price. Available techniques include ATR, diffuse reflection, specular reflection, transmission and fiber optics.

Gas cells – A variety of short- and long-pathlength gas cells are available. Cells include built-in transfer optics that fit into your spectrometer or AEM sample compartment. The cells are suitable for use in both ambient and elevated temperature conditions. Gas cell heating, transfer optics purge, gas manifold, and sample window options are available to accommodate a variety of sample gases and sampling conditions.

GC interface – This interface attaches to the right side of the spectrometer and must be connected to a gas chromatograph (GC). You can then analyze IR spectra from GC experiments using the OMNIC Series software.

Gemini – By combining two sampling technologies—horizontal attenuated total reflection (HATR) and diffuse reflection—this accessory lets you analyze a broad range of sample types. The Gemini is baseplate-mounted for high stability, and no accessory realignment is necessary when you switch sampling heads. Integral purge tubes seal the accessory from the atmosphere.

Liquid Analysis System – This system lets you collect and process quantitative analysis data for liquid samples. It uses OMNIC Integra™ software, which contains methods for quantifying components in specific types of liquids.

Microplate accessory – This accessory allows you to collect transmission or diffuse reflectance spectra of multiple solid or liquid samples consecutively. All the samples are loaded into the sample chamber at one time into a 96 or 384 well microtiter plate. The ejection, insertion, and movement of the well plate inside the sample compartment is controlled by software.

Near-IR Heated Cuvette Holder E.S.P. – This accessory is designed for analyzing samples that require a constant or elevated temperature to obtain reproducible near-IR results. You can use it to analyze liquids, gels and solids that have a low melting point, such as waxes.

PAC 300 Photoacoustic E.S.P. – Photoacoustic spectroscopy (PAS) is a powerful technique for the nondestructive spectroscopic analysis of solid samples of all types. PAS is particularly applicable to powders (including dark, highly absorbant samples), polymer pellets, beads, and sheets and films. The PAC 300 Photoacoustic E.S.P. accessory is fully integrated with the spectrometer and computer. It automatically selects an OMNIC experiment, draws power right from the spectrometer and includes an on-line tutorial.

PEM kits – A variety of PEM (photoelastic modulator) external hardware kits include a lock-in amplifier, high-pass filter, the PEM, transmission and grazing angle sample holders, a polarizer, transfer and focusing optics, and optical filters. These kits contain all the hardware needed to perform VCD (vibrational circular dichroism) and PM-IRRAS (polarization modulation infrared reflection absorption spectroscopy) experiments.

Polarizer – This accessory lets you control the orientation of the electric field vector of the infrared beam as it enters the sample compartment. This is particularly useful for characterization of monolayers, thin films and other sample types.



See “Using the polarizer” in the “Spectrometer Options” chapter for more information.



For information about installing and using an internal polarizer, view “Replacing the an internal polarizer” in the “Setting up experiments” book in Spectrometer Help Topics.

Remote Start accessory – This accessory adds external trigger capability to your spectrometer. With a press of the Start switch, you can control the start of data collection or coordinate the start of an external experiment.

SabIR™ – This accessory provides remote sampling capability for raw material identification, quality measurements, and sample component analysis. The system is optimized for diffuse-reflectance sampling of solids and powders. Materials may be sampled directly or indirectly through packaging materials.

Sample shuttle – A sample shuttle lets you collect background spectra without removing the sample from the sample compartment. The shuttle automatically moves the sample out of the beam path before background collection begins. Since the sample compartment cover is not opened, the system purge is maintained.

Specular reflection – Specular reflection provides a nondestructive method for measuring surface coatings without sample preparation. It can be used to analyze surface-treated metals, paints, semiconductors, and resin and polymer coatings. Specular reflection accessories can be installed in the spectrometer sample compartment or AEM.

TGA interface/TGA module – This interface is equipped with a built-in, temperature-controlled flow cell and must be connected to a thermogravimetric analysis (TGA) furnace. You can analyze the evolved gases from TGA experiments using the OMNIC Series software. The TGA interface is usually mounted in the sample compartment of an AEM; the TGA module is usually installed on the side of the spectrometer, leaving the AEM or spectrometer sample compartment free for other experiments and accessories.

Transmission E.S.P.[™] accessory – Transmission is the oldest and most efficient sampling technique in FT-IR spectroscopy and can be used for sampling liquids, gases or solids. A variety of cells and sample holders are available for transmission analysis. All can be mounted in the spectrometer sample compartment. Thermo Scientific E.S.P. (Enhanced Synchronization Protocol) technology provides continuous communication between the accessory and OMNIC to ensure that the accessory is operating correctly. This accessory, or the validation wheel (described below), is required for using an NPL or serialized polystyrene standard for validation with Thermo Scientific ValPro[™] software.

TRS kits – Each TRS (time-resolved spectroscopy) kit includes a fast transient data acquisition card, a high-speed photovoltaic MCT detector and the OMNIC SST with TRS experiments software package needed to perform a variety of time-resolved experiments. Time-resolved measurements to 10 nanoseconds are possible.

Validation wheel – The validation wheel is used with ValPro software to validate the performance of the spectrometer. The wheel automatically moves standard samples into the beam path at the appropriate times during the validation procedure. The samples are traceable to standards from the National Institute of Standards and Technology (NIST). An optional calibrated sample from the National Physical Laboratory (NPL) is also available.

System accessories

Some system accessories are installed by trained service engineers. Call Thermo Fisher if you are interested in ordering any of the following accessories.

Power line conditioner – Power line conditioners protect your spectrometer and other accessories from damage or malfunction due to voltage dropouts, transient spikes, frequency shifts or other disturbances in your electrical service.

Pure air dryer – If you have difficulty controlling moisture in your laboratory, the pure air dryer provides additional protection for the hygroscopic elements of your spectrometer. This accessory is also useful if your laboratory air supply is contaminated with volatile solvents, oil or other reactive materials.

Purge gas generator – If you do not have in-house facilities to supply compressed air or nitrogen for system purge, Thermo Fisher offers several purge gas generators.

Smart Purge Kit – This kit adds enhanced purging capability to your spectrometer. When you open the sample compartment cover or its sliding door, Smart Purge automatically increases the purge gas flow rate for a short time. This keeps water vapor, carbon dioxide and other unwanted gases out of the spectrometer while you install or remove a sample. You can then collect spectra without waiting for proper purge to be restored.

Uninterruptible power supply – An uninterruptible power supply reduces the chance of a system shutdown if power is lost.

How to cable an accessory

When you install an accessory in the sample compartment, you may need to connect one or more cables from the accessory to connectors on the rear wall of the compartment. You may also need to attach cables from other peripherals (such as computers, custom controllers or power supplies) to the accessory or from the accessory to the rear panel of the spectrometer. The instructions that came with the accessory should contain specific information on connecting that accessory.

Pass-through connectors

Your spectrometer may be equipped with pass-through connectors for use with special accessories. These connectors allow you to make accessory cable connections through the spectrometer. This eliminates the need to run cables through the seal on the sample compartment cover or out the top of the sample compartment.

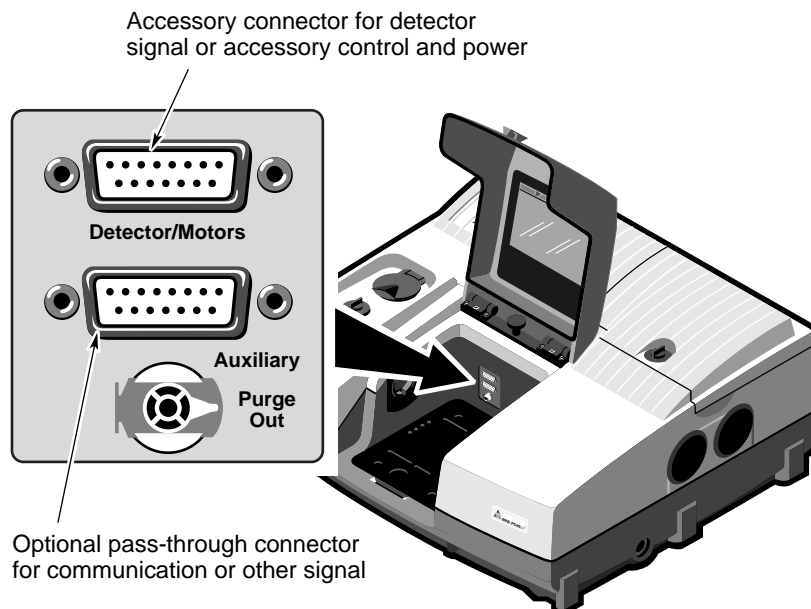
Caution

Improper or unsafe cabling can cause damage to your accessory and may create a safety hazard. Only qualified persons should cable a custom accessory using these connectors. Thermo Fisher is not responsible for damage or injury resulting from improper or unsafe cabling. ▲

To use the pass-through connectors, connect the accessory inside the sample compartment and connect the external power or communications peripheral to the corresponding pass-through connector on the rear panel of the spectrometer.

Connectors inside the sample compartment

The following illustration shows the locations of the electrical connectors inside the sample compartment.



Detector/Motors – If you have a photoacoustic or other accessory that has a detector or motor located in the spectrometer sample compartment, connect the cable from the detector or motor to this standard connector. This is *not* a pass-through connector. See “Detector/Motors connector” for information on using this connector to connect custom hardware.

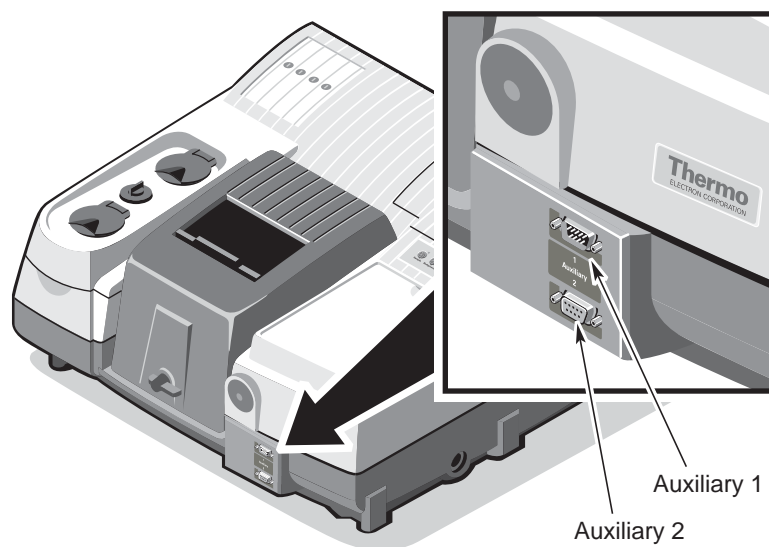
Auxiliary – Six pins on this optional connector can be used for passing DC power input or other signals from the Auxiliary 1 and Auxiliary 2 connectors on the rear panel to an accessory. For example, the automatic sample wheel and the ProfilIR accessory get DC power through this connector when the DC power output of an AC-to-DC converter is attached to the Auxiliary 1 connector on the rear panel.



See “Using connectors for custom accessories” for information on which pins are available for use.

Connectors on the front of the spectrometer

The illustration below shows the optional connectors on the front of the spectrometer that you can use to pass signals to and from the sample compartment.



Note These connectors are available only on systems that do not include the SabIR accessory or the microplate accessory. ▲

Auxiliary 1 – This connector passes power or other signals for the accessory to three pins on the Auxiliary connector inside the sample compartment. This connector could be used, for example, to attach the DC output of an AC-to-DC converter to provide DC power to an accessory in the sample compartment.

Auxiliary 2 – This connector passes signals to three pins on the Auxiliary connector inside the sample compartment. This connector could be used, for example, to allow an accessory in the sample compartment to be controlled through your computer's serial (RS-232C) port.

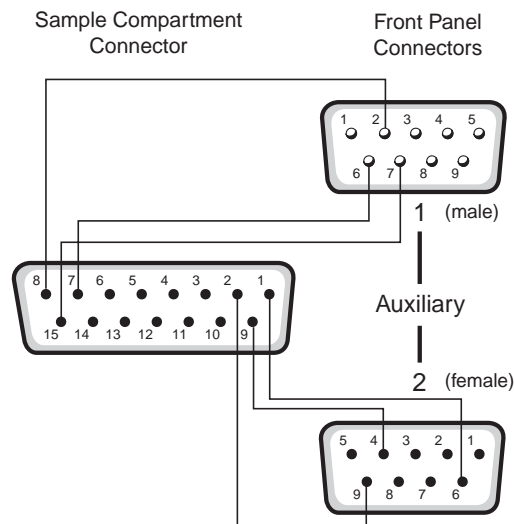
Using the pass-through connectors for custom accessories

By connecting custom cables that use the pins on the sample compartment Auxiliary, front panel Auxiliary 1 and Auxiliary 2 pass-through connectors, you can provide power and communication or other signals for your custom accessories. The power and signals pass through the spectrometer from the front to the sample compartment and vice versa. Make sure your use of the connectors complies with the following voltage and current limitations.

Warning

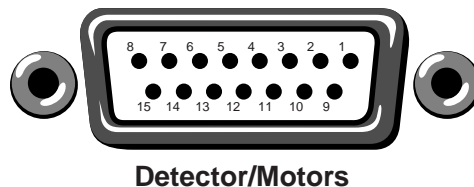
Improper or unsafe cabling can cause damage to your accessory and may create a safety hazard. Only qualified persons should cable a custom accessory using these connectors. Do not pass signals that exceed ± 15 VDC through these connectors. You must also limit the current to a maximum of 800 mA. Thermo Fisher is not responsible for damage or injury resulting from improper or unsafe cabling. ▲

The following diagram shows schematically which pins of the **Auxiliary** connector inside the sample compartment are connected *internally* to pins of the **Auxiliary 1** and **Auxiliary 2** connectors on the front of the spectrometer. Since none of these connected pins are assigned, they are available for use with custom accessories.



Detector/Motors connector

You can use the Detector/Motors connector on the rear wall of the sample compartment access power and ground for your own detectors, accessory motors and other custom hardware. Contact technical support if you wish to use the connector for control and/or communications.



⚠ Warning

Improper or unsafe cabling can cause damage to your accessory and may create a safety hazard. Only qualified persons should connect a cable to the Detector/Motors connector. Do not use this connector for signals that exceed ± 12 VDC. Limit the current to a maximum of 500 mA. Thermo Fisher is not responsible for damage or injury resulting from improper or unsafe cabling. ▲

The following table provides pinout information for the Detector/Motors connector.

Pin Number	Description
1	Reserved (do not connect)
2, 10	Reserved (sample shuttle motor control)
3, 8	+ 5 VDC
4	Analog ground
5, 7, 13, 15	Reserved (detector communications)
6, 11	+12 VDC
9	Reserved (spectrometer control)
12	Analog ground
14	-12 VDC

Answers to Your Questions About Using OMNIC

This chapter answers some common questions about using OMNIC. Each answer is followed by a reference telling you how to find more information.

Where a menu command name is given, the corresponding toolbar button is also shown. Depending on the software configuration you are using, a particular button may not be present in your toolbar.

Collecting spectra

How do I set the software for collecting spectra?



You can set the software in one step by selecting a stored experiment from the Experiment drop-down list box below the OMNIC window menu bar. To set the experiment parameters individually, use Experiment Setup in the Collect menu.

If you install a Smart Accessory, the system automatically sets the software parameters (or a list of appropriate experiments is made available for your selection), and you can begin collecting spectra.



For general information view “Preparing the Software” in the Collecting a Spectrum tutorial available through Learning OMNIC. Also, in OMNIC Help Topics find “experiment” in the Index and go to “Selecting an experiment” or “Using Experiment Setup” for a more in depth discussion.

How do I collect a spectrum?



First set the parameters as explained above. Depending on the settings, you may need to install or remove the sample before collecting data. Then press the Sample button on top of the spectrometer, or choose Collect Sample from the Collect menu.



For general information view “Collecting the Spectrum of a Sample” in the Collecting a Spectrum tutorial available through Learning OMNIC. Also, in OMNIC Help Topics find “spectrum” in the Index and go to “Collecting a sample spectrum” or “Collecting a background spectrum” for a more in depth discussion.

How do I specify the Y-axis unit for collecting spectra?



Choose Experiment Setup from Collect menu and then set Final Format on the Collect tab.



You can change the format of a collected spectrum by using Absorbance, % Transmittance or Other Conversions in the Process menu. See the question and answer in the next section for a description of the available units.



For general information view “Typical IR Transmission Spectrum” in the Collecting a Spectrum tutorial available through Learning OMNIC. Also, in OMNIC Help Topics find “units” in the Index and go to “Selecting the final format” for a more in depth discussion.

What does gain do?

Gain amplifies the detector signal intensity, making it larger relative to the level of electronic noise. This is helpful when the signal is weak, such as when you use some sampling accessories. You can let OMNIC automatically adjust the gain to maximize the signal by setting the Gain parameter to Autogain. We recommend using this setting to ensure the best spectral quality.



In OMNIC Help Topics find “gain” in the Index and go to “Setting the gain.”

When should I save interferograms with my spectra?

Save interferograms if you think you may want to restore the original data after it has been processed or if you want to keep an archive of your original data.



For general information view “Preparing the Software” in the Collecting a Spectrum tutorial available through Learning OMNIC. Also, in OMNIC Help Topics find “saving, interferograms” in the Index and go to “File handling” for a more in depth discussion.

What does the Collect Sample window show?

The window displays the “live” spectrum as it is being collected plus a gauge indicating the progress of the collection, an indicator showing whether any problems have occurred and other information about the collection.



For more information view “Collecting the Spectrum of a Sample” in the Collecting a Spectrum tutorial available through Learning OMNIC. Also, in OMNIC Help Topics find “spectrum” in the Index and go to “Collecting a sample spectrum” for a more in depth discussion.

How do I know my spectra are meeting quality standards?

OMNIC continuously monitors the quality of the data you collect, based on the parameters you set. The Quality tab in the Experiment Setup dialog box contains parameters for specifying the spectral quality characteristics that you want checked when you collect spectra.

OMNIC offers four categories of spectral quality checks:

- Spectrum checks
- Parameter checks
- Background checks
- Interferogram checks

When OMNIC performs a check and detects a problem, the Collect Status indicator is displayed as a yellow circle or a red X. Click the indicator (or click the View Collect Status button at the end of data collection) to see a summary of data collection problems encountered during the collection and other information about the collection.

When a collected spectrum passes all of the selected quality checks, the Collect Status indicator appears as a green check mark.



In OMNIC Help Topics find “quality checks” in the Index and go to “Quality checks.”

Converting spectra to other units

Which Y-axis unit should I use for a spectrum?

The most commonly used units are % transmittance and absorbance. Use % transmittance if you plan to compare the spectrum visually with published reference spectra. Use absorbance units for quantitative analysis measurements.

Kubelka-Munk units are useful for searching diffuse reflectance spectra against libraries of absorbance spectra.

Use **photoacoustic units** for spectra collected using a photoacoustic accessory.

Percent reflectance units are mathematically equivalent to % transmittance units, but using them for spectra collected using a reflection technique serves to identify the technique.

Using **log (1/R) units** for spectra collected using a reflection technique is useful for quantitative comparisons, since there is often a linear relationship between the concentration of a component and its log (1/R) value.



For general information view “Typical IR Transmission Spectrum” in the Collecting a Spectrum tutorial available through Learning OMNIC. Also, for more in depth discussions, in OMNIC Help Topics find:

- “absorbance” in the Index and go to “Converting spectra to absorbance.”
- “transmittance (%)” and go to “Converting spectra to % transmittance.”
- “Kubelka-Munk units” and go to “Kubelka-Munk units.”
- “photoacoustic units” and go to “Photoacoustic units.”
- “reflectance (%)” and go to “% Reflectance units.”
- “log (1/R) units” and go to “Log (1/R) units.”

Using spectral libraries



How do I search a spectral library?

First prepare the spectrum (as explained below) and display or select the region you want searched. Then set up the search using Library Setup in the Analyze menu and start the search by clicking the Search button in the Library Setup dialog box or by choosing Search from the Analyze menu.



In OMNIC Help Topics find “library” in the Index and go to “Setting up a library search” or “Searching a spectral library.”

How can I display a library spectrum in a spectral window?



If you are using OMNIC, locate and select the spectrum in Library Manager (available through the Analyze menu) and then click the Add To Window button, or go to the Library Spectra tab of Library Manager, display the desired spectrum on the tab and then double-click the spectrum.



In OMNIC Help Topics find “library” in the Index and go to “Working with libraries.”

How should I prepare my spectrum before searching it against a spectral library?

There are several corrections you can perform on a spectrum to obtain the best search results:



- If the baseline of the spectrum is sloped, curved or shifted vertically, correct it using Baseline Correct in the Process menu.



- If the spectrum has totally absorbing bands, eliminate them by using Blank in the Process menu. Be careful not to blank regions that contain other important spectral information.
- You can also use the region tool to select a region of the spectrum that does not include any totally absorbing bands or use the view finder to display the region before searching. (These methods avoid the loss of spectral information that results from blanking.)
- If you collected the spectrum using specular or diffuse reflection, use Kramers-Kronig (dispersion) correction (available through Other Corrections in the Process menu) to correct it for dispersion effects and then search it against a library of absorbance spectra.
- If the spectrum has water or carbon dioxide peaks, use Other Corrections to remove these peaks.



In OMNIC Help Topics find:

- “baseline” in the Index and go to “Correcting a baseline manually.”
- “blanking spectral region” in the Index and go to “Blanking a spectral region.”
- “spectral region” in the Index and go to “Region tool” or “View finder.”
- “Kramers-Kronig transformation” in the Index and go to “Kramers-Kronig (dispersion) transformation.”
- ATR correction” in the Index and go to “ATR correction.” “water” in the Index and go to “H2O and CO2 correction.”

Only those portions of the spectrum which are within the selected region (or displayed region if no region is selected) and within any of the regions you specified for the library using the Region Setup tab of the Library Setup dialog box will be included in the search. If the spectral range of the spectrum is broader than that of the library spectra, use the region tool to select the region of the spectrum that coincides with the library spectra before you start the search. You can also use the view finder to display the region to search. The Search command operates on the selected region, or on the displayed region if a region is not selected



In OMNIC Help Topics find “spectral region” in the Index and go to “Region tool” or “View finder.”

How do I create a spectral library?



If you are using OMNIC, use the Create Library button on the Library Names tab of Library Manager (available through the Analyze menu) to create a user library.



Once a library is created, you can add spectra to it with Add To Library in the Analyze menu or by dragging the spectrum to the library’s book on the Library Names tab of Library Manager. You can use a search library you create just as you would a commercial library to identify unknown spectra. You can use a QC library to verify the composition of a sample. If you create a scrapbook library, you can find spectra in it by searching for text (but not by spectral searching)

When you create a library, you determine the kinds of information that will be saved with it.



In OMNIC Help Topics find “library” in the Index and go to “Creating a user library” and “Adding spectra to a user library.”

How do I create a spectral library?



If you are using OMNIC, use the Create Library button on the Library Names tab of Library Manager (available through the Analyze menu) to create a user library.



Once a library is created, you can add spectra to it with Add To Library in the Analyze menu or by dragging the spectrum to the library's book on the Library Names tab of Library Manager. You can use a search library you create just as you would a commercial library to identify unknown spectra. You can use a QC library to verify the composition of a sample. If you create a scrapbook library, you can find spectra in it by searching for text (but not by spectral searching).

When you create a library, you determine the kinds of information that will be saved with it.



In OMNIC Help Topics find “library” in the Index and go to “Creating a user library” and “Adding spectra to a user library.”

How can I find a compound in a commercial library?



If you are using OMNIC, Library Manager in the Analyze menu lets you search for the compound name. After you select the library on the Library Names tab, use the features on the Search For Text tab to locate the spectrum. Type the text to search for in the Text In Selected Item box, and then choose Search. The search results appear in the table based on the options you have set. To see information about a found spectrum, double-click its row in the table.



In OMNIC Help Topics find “library” in the Index and go to “Searching a library for text.”

You can use the extended search feature (available on the Extended Search tab of the Library Setup dialog box) to find library spectra by searching for text in any field included in the library. For example, some libraries have fields for molecular weight, boiling point or manufacturer.



In OMNIC Help Topics find “extended search” in the Index and go to “Using extended search.”

What is the easiest way to collect sample spectra and add them to a spectral library?



If you are using OMNIC, use the Collect Spectrum button on the Library Names tab of Library Manager (available through the Analyze menu) to collect a spectrum and add it to a user library. The software automatically sets the experiment parameters (for example, Resolution) so that the spectrum will be compatible with the selected library. This allows you to collect and add a compatible spectrum in one step instead of three (using Experiment Setup to set the parameters, Collect Sample to collect the spectrum and Add To Library to add the spectrum to the library).

What does the search expert do?

It determines the search algorithm to use, searches the spectral region from 2600 to 450 wavenumbers and then displays the specified number of library spectra that best match the unknown spectrum, plus comments about the search results. For example, the search expert may tell you that the best match is excellent but the second best match is also similar to the unknown. You will be able to display the list of matches to see their match values and index numbers.

Opening, saving and deleting spectra



How do I open a stored spectrum?

Choose Open from the File menu, locate the spectrum or spectra you want to open, select the filenames of the spectra and then choose OK. You can hold down the Control key to select multiple files.

In OMNIC Help Topics find “spectrum” in the Index and go to “Opening spectra.”

How can I save my collected spectra automatically?



Choose Experiment Setup from the Collect menu and turn on Save Automatically on the Collect tab (Save Automatically is on by default). Specify a base name for naming the saved spectral data files in the Base Name box. A sequential number will be appended to the base name when the spectra are saved. If you want the interferograms saved with the spectra, turn on Save Interferograms. Individual spectra are saved with the extension .SPA.



In OMNIC Help Topics find “saving, spectra” in the Index and go to “File handling.”

You can also view “Preparing the Software” in the “Collecting a Spectrum” tutorial (available through Learning OMNIC in the Help menu).

Where should I save my spectra?

You have several options for saving spectra; you may choose to use more than one.

For a permanent record of the spectrum and any other information you want to record, use a report notebook.



In OMNIC Help Topics find “report notebook” in the Index and go to “Adding a report to a notebook.”

You can also place spectra in descriptively named user libraries that you create. Keeping spectra in libraries allows you to find them by searching for text contained in the information saved with the spectra.



In OMNIC Help Topics find “spectrum” in the Index and go to “Adding a spectrum to a user library.”

Note

When you add a spectrum to a user library whose resolution is lower, the spectrum is deresolved. To maintain the original data, save your sample spectrum as a file. Make a copy of the file and then add the copy to the lower resolution library. The lower resolution data would be used for searching purposes only. ▲

We recommend that you create descriptively named folders (directories) on your hard disk for different categories of spectra. For example, you could have a folder for each project you are working on, for each of your clients, for each laboratory application, or for each sample type. See your Windows documentation for information about creating directories. You can specify which folder to use when you use Save or Save As in the File menu to save spectra. This will make it easier to find a spectrum in a particular category when you use Open in the File menu to open a spectrum.



In OMNIC Help Topics find “spectrum” in the Index and go to “Saving spectra using new filenames.”

How can I save several spectra in one file as a group?



Select the spectra and then choose Save Group from the File menu. To select more than one spectra, hold down the Control key and click each spectrum you want to select with the selection tool, and then release the Control key. Spectral groups are saved with the extension .SPG.



In OMNIC Help Topics find “saving, spectra” in the Index and go to “Saving a group of spectra.”

How can I delete stored spectra?



Choose Delete Files from the File menu to display the Delete Files dialog box. Locate and select the spectral data files (with the extension .SPA, or .SPG for spectral group files) you want to delete and then choose OK.



In OMNIC Help Topics find “spectra” in the Index and go to “How to delete files.”

Can I delete an entry from a report notebook?

No. OMNIC’s report notebooks are similar to traditional laboratory notebooks in that information you add to them becomes part of the permanent record of your work.



You can delete an entire notebook, however, by deleting the entire notebook file. Choose Delete Files from the File menu to display the Delete Files dialog box. Locate and select the directory containing the notebook data files (with the extension .NBK). You will have to set the List Files Of Type box to *.NBK or All (*.*) to see the notebook data files. Select the file(s) you want to delete and then choose OK.

Printing

How can I specify a printer for printing information?



Use Printer Setup in the File menu. See your Windows documentation for details on setting the printer parameters.



In OMNIC Help Topics find “printer” in the Index and go to “Setting up the printer.”

How can I create and print reports of my work?

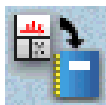


Use the commands in the Report menu. First use Template to select, edit or create a template for the report. Then use Preview/Print Report to view the report as it will appear on paper. Click the Print button to print the report.



View Creating Reports (available through Learning OMNIC) for more detailed information about OMNIC reports.

Also, in OMNIC Help Topics find “template” in the Index and go to “Selecting, editing or creating a report template,” or find “report, previewing or printing” and go to “Previewing or printing a report.



You also can use Add To Notebook to add the report to a report notebook. You can then print the report with the Print button when you view the notebook using View Notebook..



In OMNIC Help Topics find “report” in the Index and go to “Adding a report to a notebook.

How can I preview spectra or other information before printing?

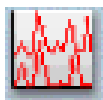
Use Preview/Print Report in the Report menu to view a report as it would appear on paper. The report is displayed using the current report template; that is, the template you specified with Template or the one you are viewing and working with. If the report is displayed as you want it to appear on paper, you can print it by using the Print button.



In OMNIC Help Topics find “template” in the Index and go to “Selecting, editing or creating a report template,” or find “report, previewing or printing” and go to “Previewing or printing a report.”

Displaying spectra

How can I select more than one spectrum at a time?



After selecting the first spectrum by clicking it, hold down the Control key while you click each additional spectrum. You can also choose Select All from the Edit menu to select all the spectra in the window that are not hidden.



In OMNIC Help Topics find “spectra” in the Index and go to “Selection tool” or “Selecting all the spectra in a spectral window.”

How can I specify colors for displaying spectra?



Choose Options from the Edit menu, click the View tab and then choose Colors. In the Colors dialog box click the color next to the spectrum number for which you want to specify the color and then click the desired color in the color array. To specify the color for selected spectra, click the color next to Selected Spectrum and then click a color. Typically red is the color reserved for displaying selected spectra.



In OMNIC Help Topics find “spectra” in the Index and go to “Specifying colors for spectra and other features.”



You can also specify colors for displaying spectra in a particular spectral window. Start by selecting the spectra for which you want to specify a color, and then choose Display Setup from the View menu. Click the desired color in the color array and then choose OK. When the spectra are no longer selected, such as after you select a different spectrum, they will be displayed in the color you clicked.



In OMNIC Help Topics find “spectra” in the Index and go to “Selecting a color for the currently selected spectra.”

What is the difference between the Display Setup parameters and the Window options?



The parameters in the Display Setup dialog box affect the currently active spectral window only. The options in the Window options (in the Options dialog box, available through the Edit menu) affect all the new spectral windows that you create. After you create a new spectral window, you can change the way spectra are displayed in it by using Display Setup in the View menu.



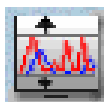
In OMNIC Help Topics find “display parameters” in the Index and go to “Setting the display parameters,” or find “Window options” and go to “Window options.”

What can I do with the “Scale” commands in the View menu?

You can display spectra so that they are easier to see or compare.



Full Scale displays the spectra so that they perfectly fit their panes vertically. Automatic Full Scale does this automatically when you change the display with the view finder or selection tool. The Y-axis displayed corresponds to the selected spectrum.



Common Scale displays all the spectra so that they are not cut off at the top or bottom and use the same Y scale. This allows you to compare the band intensities of different spectra.



Match Scale changes the Y scale of the spectra to be the same as that of the selected spectrum. (The selected spectrum’s scale is not changed.) This allows you to compare the band intensities of different spectra.



Offset Scale shifts the spectra vertically so that they overlap less, making them easier to see.

When you use these commands, keep in mind that the current Y-axis is always accurate for the currently selected spectrum but may not apply to other spectra in the window.



For a more detailed discussion, in OMNIC Help Topics find “spectra” and go to:

- “Displaying spectra full scale” or “Displaying spectra full scale automatically.”
- “Displaying spectra using the same Y-axis.”
- “Matching the Y scale of a spectrum.”
- “For information about Offset Scale, find “spectra” and go to “Displaying spectra vertically offset.”

How can I zoom in on an area of a spectrum?



Draw a box around the area using the selection tool and then click inside the box.



You can also use the Expand/Contract buttons at the left end of the view finder or drag the regions markers in the view finder to display a smaller spectral region. You can press and hold down the mouse button during these operations to continuously expand or contract the display.

To expand and contract the spectra horizontally about the center, use the view finder's Horizontal Expand/Contract buttons (left-most). To expand and contract the spectra vertically about the center, use the Vertical Expand/Contract buttons (right-most).



The Roll/Zoom Window in the View menu also expands or contracts an area. In OMNIC Help Topics find “Roll/Zoom Window command” in the Index and go to “Rolling and zooming spectra” for more information about expanding and contracting a spectral region.

How can I move a spectrum up or down in its pane to see it better?



Use the selection tool to drag the spectrum up or down. The Roll/Zoom window available in the View menu to move a spectrum up or down.



In OMNIC Help Topics find “Roll/Zoom Window command” in the Index and go to “Rolling and zooming spectra” for more information about moving spectrum.

How can I move a spectrum into another spectral window?



Use the selection tool to drag the spectrum from one spectral window to another. A copy of the spectrum appears in the second window, and the original spectrum remains in the first window. You can also copy or cut the spectrum using Copy or Cut in the Edit menu and then paste it into another spectral window using Paste.



In OMNIC Help Topics find “spectrum” in the Index and go to “Selection tool,” or find “pasting, spectrum” and go to “Pasting items.”

How can I move a stacked spectrum into another pane?



Use the selection tool to drag the spectrum from one pane into another.



In OMNIC Help Topics find “spectrum” in the Index and go to “Selection tool” for more information.

How can I find the X and Y values of a point in a spectrum?



Use the spectral cursor tool to click the point. The values are displayed in the readout above the palette



In OMNIC Help Topics find “X and Y values” in the Index and go to “Spectral cursor tool.”

How can I find the height of a peak?



Use the peak height tool to click the top of the peak. Then drag the baseline handles to adjust the baseline used for the measurement. The corrected (measured above the baseline) and uncorrected height values appear in the readout above the palette.



In OMNIC Help Topics find “peak” in the Index and go to “Peak height tool.”

How can I find the area of a peak?



Use the peak area tool to drag across the peak. Then drag the baseline handles to adjust the baseline used for the measurement. The corrected (measured above the baseline) and uncorrected area values appear in the readout above the palette.



In OMNIC Help Topics find “area” in the Index and go to “Peak area tool.”

Correcting spectra **Should I correct the baseline of my spectrum?**

If a baseline is sloped or curved or significantly above zero absorbance (or below 100% transmittance), a likely cause is how the sample was prepared. By correcting the baseline, you can often avoid having to prepare the sample again and collect a new spectrum.

Correcting a baseline will give you better results when you search the spectrum against a library, subtract the spectrum from another spectrum, find peaks in the spectrum or quantify components in the spectrum.



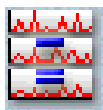
For more detailed instructions view “Common Problems with IR Spectra” in Collecting a Spectrum , available through Learning OMNIC.

In OMNIC Help Topics find “baseline” in the Index and go to “Correcting a baseline manually.”

Using spectral math

How can I subtract a spectrum from another spectrum?

Use Subtract in the Process menu whenever you want to subtract one spectrum from another. Subtract is commonly used to remove spectral features of solvent residues or pure components from the spectrum of a mixture of compounds. Subtract is available only when two spectra are selected.



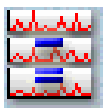
Select the spectrum from which you want to subtract spectral features; this is the sample spectrum. Then hold down the Control key and select the spectrum with the features you want to subtract from the sample spectrum; this is the reference spectrum.

Choose Subtract from the Process menu. The difference spectrum is displayed full scale in the bottom pane. This spectrum is the result of subtracting the reference spectrum from the sample spectrum using the subtraction factor shown to the left of the result. If you are not satisfied with the subtraction result, you can change the subtraction factor.



In OMNIC Help Topics find “spectrum” in the Index and go to “Subtracting spectra.”

What should I use subtraction for?



Subtract is commonly used to remove spectral features of solvent residues or pure components from the spectrum of a mixture of compounds. When you use Subtract, the software calculates data point by data point the difference between the two.

Spectral subtraction is useful in a variety of situations, for example..

- Eliminating solvent peaks in a spectrum of a sample that is dissolved in a solvent.

- Separating components from a sample that is a mixture of two or more components.
- Identifying an unknown contaminant by subtracting out the known sample material.
- Ensuring quality by subtracting an original batch sample spectrum from a spectrum from the next batch.

What other mathematical operations can I perform on my spectra?



You can manipulate spectra using any of the common math operations. Use Spectral Math in the Process menu to perform these operations on one or two selected spectra. You specify the operations to perform by typing a sequence of mathematical symbols and numbers. The software performs the operations on the Y values of the data points in the spectrum or spectra and then displays the result spectrum.

When you choose the command, the Spectral Math window appears allowing you to type the desired operations in the Operation text box. You can also select one of the example operations provided in the Operation drop-down list box.



View Using Spectral Math (available through Learning OMNIC) for more detailed instructions.

Also, in OMNIC Help Topics find “spectrum” in the Index and go to “Performing arithmetic operations on spectra.”

Customizing OMNIC



How can I customize my OMNIC software?

You can use Options in the Edit menu to set options that determine how the software operates. You can also customize the menus and the toolbar using Edit Menu and Edit Toolbar in the Edit menu.

Use Save Configuration As in the File menu to save your customized settings in a configuration file. You can then open the file later to reset OMNIC to your preferences in one step.

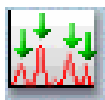
View “Preparing the Software” in Collecting a Spectrum (available through Learning OMNIC) for more detailed instructions.

Also, in OMNIC Help Topics find:

- “options” and go to “Customizing OMNIC by setting options.”
- “menu” and go to “Customizing a menu.”
- “toolbar” and go to “Customizing a toolbar.”
- “configuration” and go to “Opening a configuration” and “Saving a configuration.”

Other questions

How can I find and label peaks in spectra?



Use Find Peaks in the Analyze menu to find and label peaks above a specified threshold.



You can also use the annotation tool to label individual peaks



In OMNIC Help Topics find “peaks” in the Index and go to “Finding peaks above a specified height,” or find “label” and go to “Annotation tool.”

How can I close a task window (such as the Find Peaks window)?



Click the Close button (if available) in the upper-right corner of the window. You can also double-click the button at the left end of the window’s title bar (if the window is *not* maximized) or the button at the left end of the menu bar (if the window is maximized).



In OMNIC Help Topics find “task window” in the Index and go to “Task windows.”

How can I select a spectral region for an operation?



Use the region tool to drag across the region in the pane.



In OMNIC Help Topics find “spectral region” in the Index and go to “Region tool.”

How can I display information about how a spectrum was collected and processed?



Select the spectrum and then click the Information button to the left of the title box. You can also double-click the spectrum's title in the title box.



In OMNIC Help Topics find “collection and processing information” in the Index and go to “Collection and processing information.”



If you want this kind of information displayed in a spectrum's pane, choose Display Setup from the View menu, turn on Sampling Information and then specify the types of information you want displayed by turning on options in the Sampling Information box.



In OMNIC Help Topics find “displaying, sampling information” in the Index and go to “Displaying sampling information.”

How can I copy a spectrum and paste it into a text document?



Select the spectrum and choose Copy from the Edit menu. This places the spectrum on the Clipboard in the form of a Windows metafile (this is the file format with the most flexibility for pasting into other programs). You can then paste the spectrum into a document by using a word processing program.



In OMNIC Help Topics find “copying, spectrum” in the Index and go to “Copying items.”

How can I get on-line Help while using the software?

The OMNIC on-line Help system lets you quickly find answers to your questions about using the software. There are several ways to enter the Help system:

- To see information about a particular control or drop-down menu item in OMNIC, click the item using the right mouse button. A brief description appears and, in most cases, one or more buttons that you can click to display more detailed information. Click the Discussion button to display a complete discussion of the control, menu item (or the dialog box / window that contains the control). Click the How To button to display a step-by-step procedure for using the feature (or the dialog box or window that contains the feature).
- You can press the F1 function key at any time to see a discussion topic for the currently displayed or selected menu item, control, dialog box or window.
- If a dialog box or window contains a Help button, click it to see information about the dialog box or window (or the command that displayed it).
- Choose a Help system or tutorial from the Help or SST menu.
- Choose Advanced Applications from the SST menu.

Answers to Your Questions About Using the Spectrometer

This chapter answers some common questions about using your spectrometer. Each answer is followed by a reference telling you where to go for more information.

Do I need to use an energy screen with my detector?

If you are using a highly sensitive detector such as a PbSe, Si, MCT-A or InSb detector and your experiment deals with information from a broad range of frequencies, use an energy screen to prevent the detector from becoming saturated or producing a distorted signal.



In Spectrometer Help Topics find “Installing an energy screen” in “Setting up experiments.”

When do I need to open the spectrometer cover?

You need to open the spectrometer cover to change sources. Also, you need to open the cover if you are installing a spectrometer component such as a laser.



In Spectrometer Help Topics find “Opening the main cover” in “Installing optional hardware.”

⚠ Warning

Do not operate the spectrometer with the main cover open. The cover protects you from exposure to laser light and live electrical connections. If you must open the main cover for maintenance or service reasons, always turn the spectrometer power off first. ▲

When should I align the spectrometer?

Align the spectrometer after you install a new beamsplitter, replace the laser or move the spectrometer. It is also a good idea to align the spectrometer if the signal intensity has dropped significantly from its usual level. For best performance align the spectrometer at least once a week (once a day if you are performing step-scan or other advanced experiments).



In Spectrometer Help Topics find

- “Changing the beamsplitter” in “Setting up experiments.”
- “Changing detectors” in “Setting up experiments.”
- “Replacing the source” in “Replacing Parts.”

In OMNIC Help Topics find “aligning, spectrometer” in the Index and go to “Aligning the spectrometer.”

Does my detector need to be cooled with a cryogen?

Detectors that have a dewar need to be cooled. Dewar detectors are fairly large metal cylinders with a hole in the top. These include MCT and InSb detectors. To determine if your detector requires cooling, open the detector compartment cover and see if the detector has a dewar.

If during a work session you find that the signal intensity from your cooled detector is decreasing, it may need to be refilled with liquid nitrogen. With proper care, a detector dewar should maintain its insulating vacuum for several years. If the vacuum leaks, the insulation will lose effectiveness and the following symptoms may occur

- Liquid nitrogen boils off much faster than usual
- The outside of the dewar stays cold more than 30 minutes after filling and may feel damp or become frosted
- Water and atmospheric contaminants condensing on the detector window show up in spectra as unwanted peaks

Notice If the detector dewar loses vacuum, restore the vacuum as soon as possible. Leaving the detector elements exposed to atmospheric pressure can damage them. ▲

If you suspect that the detector dewar has a vacuum leak, contact technical support.



In Spectrometer Help Topics find “Cooling a detector” in “Setting up experiments” and “Restoring the dewar vacuum” in “Troubleshooting.”

When should I change the desiccant (in sealed and desiccated spectrometers only)?

If your spectrometer is in use:

Check the performance of the desiccant by using the Check Desiccant button on the Diagnostic tab of the Experiment Setup dialog box. If the check indicates that the desiccant is no longer effective, replace it.

If your spectrometer is in storage:

Check the round, blue indicator on the desiccant holder under the beamsplitter compartment cover monthly. Change the desiccant if the indicator has turned pink.



In Spectrometer Help Topics find “Checking and changing desiccant” in “Maintaining your spectrometer.”

Also, see the replacement parts lists in “Ordering Parts” in Spectrometer Help Topics to find the part number for desiccant bags. The desiccant holder under the beamsplitter compartment cover holds one bag.

Which source should I use?

Use the source that is appropriate for the spectral range of your experiment (determined by the ranges of the beamsplitter and detector). Thermo Fisher offers a mid-IR to far-IR source (Ever-Glo) and a near-IR source (white light).



In OMNIC Help Topics find “source” in the Index and go to “Specifying the source type.”



In the “Spectrometer Basics” chapter, see “Selecting the right source, beamsplitter and detector” in “Using beamsplitters and detectors.”

Should I turn off the spectrometer when I’m not using it?

We recommend that you leave the spectrometer on. This improves the thermal stability of the system and gives you more consistent results when you collect spectra.

How can I diagnose problems with the spectrometer?

The performance of the spectrometer is monitored while you collect spectra. If a problem occurs, a troubleshooting message appears.



In Spectrometer Help Topics see the “Troubleshooting” book for instructions on diagnosing spectrometer problems and ordering and replacing parts.

Note

If you want to view the on-line videos to help you in troubleshooting a problem, put the Spectrometers Tutorials CD in the computer. ▲

You can also make a more thorough check on a spectrometer component by choosing Advanced Diagnostics from the Collect menu. This starts the Bench Diagnostics program, which provides information on the status of the component as well as troubleshooting information, replacement procedures and information on ordering replacement parts.



In Spectrometer Help Topics see the “Troubleshooting” book for instructions on diagnosing spectrometer problems and ordering and replacing parts.

In OMNIC Help Topics find “diagnostics” in the Index and go to “Checking bench components.”



See the “Diagnostics” chapter later in this manual.

How do I replace parts in the spectrometer?



See “Replacing parts” in Spectrometer Help Topics.

Maintenance and Service

This chapter describes maintenance and service routines that you can perform on the spectrometer. We define maintenance as an occasional procedure you perform to keep the spectrometer running efficiently. We define service as a procedure to replace a failing part in the spectrometer.

Warning

Perform *only* those procedures described in this chapter. If there are other problems, contact technical support. ▲



See the “Troubleshooting” book in Spectrometer Help Topics for instructions on diagnosing spectrometer problems and ordering and replacing parts.

View “Maintaining your spectrometer” in Spectrometer Help Topics for instructions for common maintenance procedures, such as changing desiccant, cleaning the purge filter and cleaning the outside of the spectrometer.

Aligning the spectrometer and accessories

To ensure optimum system performance (high signal intensity, low noise and good sensitivity), you should occasionally align the spectrometer using the OMNIC software. This section describes how to use the OMNIC software to align the spectrometer and accessories.



See the “Troubleshooting” book in Spectrometer Help Topics for instructions on diagnosing spectrometer problems and ordering and replacing parts.

Aligning the spectrometer

If you have just turned on or moved the spectrometer, wait 15 minutes (one hour for best results) before you align it so that it will have time to stabilize.

To align the spectrometer:

- 1. Remove any sample or accessory from the sample compartment.**

The beam path must be clear during alignment. Open the sample compartment as briefly as possible to maintain a constant purge.

- 2. Choose Experiment Setup from the Collect menu.**

The Experiment Setup dialog box appears.

- 3. Make sure Sample Compartment on the Bench tab is set to Main.**

- 4. Set Gain on the Bench tab to 1.**

Do not use Autogain.

An interferogram is shown in the live display. If you want to view a single-beam spectrum instead, turn on the Single Beam check box below the live display.

If you want to hear a tone whose pitch indicates the signal intensity, turn on the Tone check box below the live display. The tone reaches its highest pitch when the signal is maximized.

5. To perform an alignment, click the Align button on the Diagnostic tab.

When you click the Align button, the system begins to optimize the detector signal for maximum energy throughput. Alignment should take 2 to 4 minutes.

The live display of the detector signal changes as each interferogram is collected. The positive peak and negative peak intensities are shown next to Max and Min above the live display. The interferogram location will be shown next to Location, unless you turned on Single Beam.

6. When the alignment is finished, close the Experiment Setup dialog box.

Aligning an accessory

You also can align accessories that mount inside a sample compartment. First align the spectrometer without the accessory installed, as described above. Then set Sample Compartment on the Bench tab of the Experiment Setup dialog box according to the accessory location. Set Gain to a value that gives a signal intensity that is appropriate for the accessory. ATR and diffuse reflection accessories typically use a Gain setting of 2 or 4

If you are not satisfied with the signal intensity after alignment, you can manually align most accessories to maximize the signal. For complete instructions, see the manual that came with the accessory.

When you manually adjust an accessory, watch the largest interferogram peak. The larger this peak, the better is the signal intensity.

Note The largest interferogram peak can be positive or negative. ▲

If you are unable to see the display, turn on Tone before adjusting the accessory. The tone reaches its highest pitch when the signal is maximized.

Servicing your spectrometer

Three spectrometer components—the light source, the laser module and the main power supply—were designed so you can replace them yourself if they fail.

Note The diagnostics software will alert you to failing components. For instructions on diagnosing spectrometer problems, ordering parts and replacing parts, choose Spectrometer Help Topics from the Help menu. ▲

If the source, laser module or power supply must be replaced, refer to the replacement parts list available in Spectrometer Help Topics from the Help menu.

Diagnostics

This chapter explains how to use diagnostic software features to find and correct problems that occur when you use the system. We will cover:

- Checking the performance of spectrometer components.
- Running the spectrometer performance test.
- Performing advanced diagnostic tests.

Checking spectrometer components

OMNIC continuously monitors the operation of the spectrometer hardware and shows its status with the Bench Status indicator below the menu bar of the OMNIC window. If your system is not performing properly, you can use the Diagnostic tab in the Experiment Setup dialog box to check the performance of spectrometer components and determine the source of the problem.

Note If the noise readings are greater than normal or have changed significantly, call the technical support for assistance. ▲

To check spectrometer components and run performance tests:

1. Make sure the main sample compartment is empty.

Remove any samples and sampling accessories.

2. Choose Experiment Setup from the OMNIC Collect menu.

The Experiment Setup dialog box appears.

3. Click the Diagnostic tab.

The Diagnostic tab appears showing icons for the major components of the spectrometer with a live display of the signal from the detector.

4. To run the diagnostic tests for a component, click that component's indicator icon.

A dialog box appears showing the status of the component. If the operating values for the component are within proper limits, a check mark appears in the Status column. If the value is outside the acceptable range, an X appears in the Status column.

When you are finished viewing the information, choose OK.

5. Click the Performance Tests button and follow the instructions that appear on the screen.

If special performance tests are available for your spectrometer, a button labeled "Extended Tests" (or another appropriate name) will appear. Click this button and follow the instructions that appear on the screen to perform the tests.

Advanced diagnostic tests

The diagnostics software provided with your system lets you perform advanced diagnostic tests on the main components of the spectrometer. You should run these tests if you have problems with your spectrometer to determine the source of the problem. The diagnostics provide information on the status of the component as well as troubleshooting information, replacement procedures and information on ordering replacement parts.

Use the advanced diagnostics software to:

- Run the spectrometer signal-to-noise test.
- Test specific components of your spectrometer.
- Check the spectrometer configuration.
- Get additional troubleshooting tips.

The Bench Diagnostics program includes performance tests for step-scan and dual-channel experiment, rapid-scan, and the expanded spectral range circuits available with your spectrometer.

Follow these steps to run the advanced diagnostics:

1. Make sure the main sample compartment is empty.

Remove any samples and sampling accessories.

2. Start the diagnostics software.

To do this, choose Advanced Diagnostics from the Collect menu. You can also click the Start button in Windows, point to Programs, point to the OMNIC folder and then choose Bench Diagnostics. Some of the advanced features of the software, including the performance test, are not available if you run the diagnostics from OMNIC.

3. Follow the directions that appear on the screen to run the diagnostic tests.

When you are finished viewing information in a window, you can use the navigation buttons to return to earlier windows. Click this button to return to the previous window.



Click this button to return to the main Diagnostics window.



Exit the diagnostics software by clicking the Close button at the far right end of the title bar.

Preparing for advanced tests

If you plan to test the visible capabilities, make sure the quartz beamsplitter, silicon detector and appropriate energy screen or optical filter are installed in your spectrometer and selected (using Experiment Setup) before you start the Bench Diagnostics.

Follow these steps to test these capabilities:


- 1. Remove any samples or accessories from the sample compartment.**
- 2. Use Experiment Setup in the Collect menu to select the beamsplitter you need for your tests.**

If you are planning to run one of the visible tests, select the quartz beamsplitter.

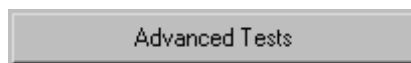
- 3. Exit OMNIC.**
- 4. Start the Bench Diagnostics.**

Choose Start, point to Programs and then choose Bench Diagnostics in the OMNIC folder.

- 5. Choose Performance Test.**

A rectangular button with a grey background and a thin black border. The text "Performance Test" is centered on the button in a black, sans-serif font.

6. Choose Advanced Tests.



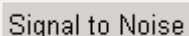
7. Click the button labeled with the name of the test you wish to run.

Note Some tests are available only when the optional software is installed on your computer. ▲

About the individual tests

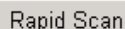
The Advanced Tests button provides access to a signal-to-noise test and performance tests for step-scan experiments, dual-channel experiments, rapid scan, and the expanded spectral range capabilities of your spectrometer.

Signal-to-noise



You can use the signal-to-noise test to track long-term spectrometer performance. Run it after you install the system and then weekly. Keep a record of the actual noise ratio values obtained. When you run the test, the software measures the response of the spectrometer optics and atmospheric absorptions in the spectrometer and then collects a “sample” spectrum with no sample in place. The result is a “100% line,” a display of system noise that appears as a generally flat line at 100% transmittance.

Rapid scan



When you choose Rapid Scan, the diagnostic checks the number of scans per second at the highest linear scan velocity for your spectrometer. The results are reported as number of scans per second and indicate whether the spectrometer passed or failed the test.

Visible




Two visible spectral range tests are available. The description adjacent to each button identifies the capabilities tested when you choose a Visible test.

You must install and select a quartz beamsplitter and silicon detector before these tests are enabled. You also will need to install a blue filter.

- Use the broad-band blue filter when testing the 23,000 to 16,000 cm^{-1} capabilities.
- Use the narrow-band blue filter when testing the 25,000 to 23,000 cm^{-1} capabilities.



See “Installing optional hardware” in Spectrometer Help Topics for complete instructions for installing detectors, beamsplitters and filters.

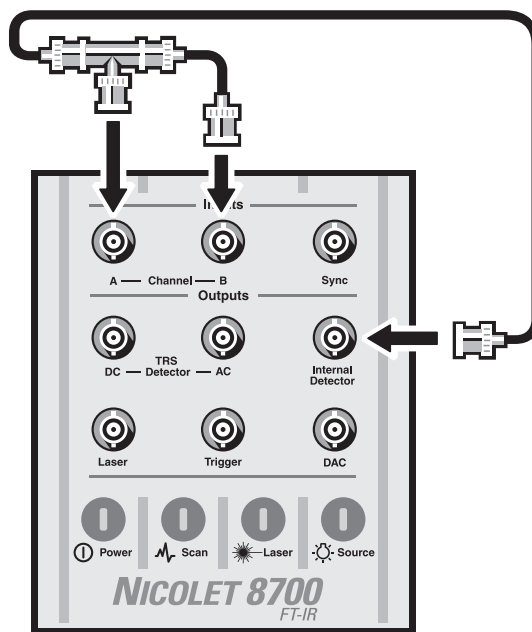
Dual-channel



Choose PEM to test the dual-channel circuitry. You do not need to set any data collection parameters before running this test. However, you may need to reset the parameters before running your next dual-channel experiment.

You must install cables before using this test.

1. **Install a BNC “T” connector on the Channel A input.**
2. **Use BNC-to BNC cables and connect the Channel B input and the Internal Detector to the Channel A input.**



Step-scan

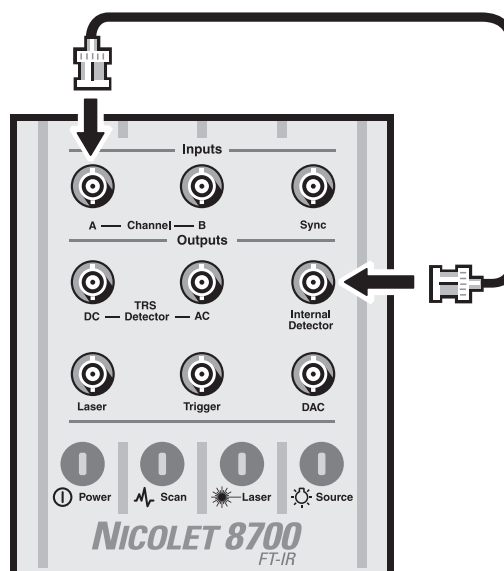
The step-scan data collection circuitry can be tested for a variety of modes.

Amplitude modulation

AM Step Scan

Choose AM Step-Scan to test the step-scan amplitude modulation circuitry. You do not need to set any AM setup parameters before running this test. Your parameters will be restored when the test is completed. You must install a cable and an energy screen before using this test.

1. **Connect a BNC-to-BNC cable between the Channel A input and Internal Detector output connectors on top of the spectrometer.**

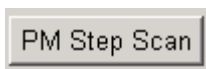


2. Install energy screen B in the sample compartment.



In Spectrometer Help Topics view “Installing an energy screen” in the “Setting up experiments” book for instructions on installing energy screens.

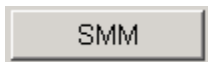
Phase modulation



Choose Step-scan PM to test the phase modulation step-scan circuitry in the spectrometer and reports the signal-to-noise ratio.

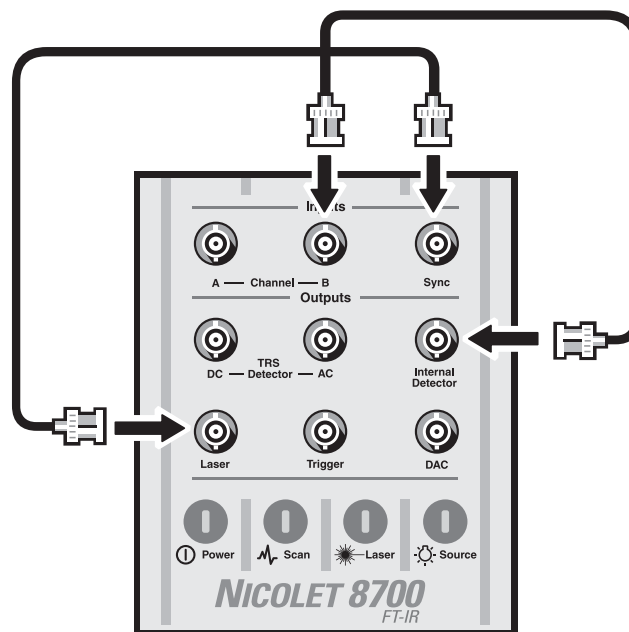
No cable connections are required. You do not need to set any phase modulation data collection parameters before running this test. Your parameters will be restored when the test is completed.

Multiple modulation



Choosing SMM runs a simulation of a multiple modulation experiment. It verifies the basic operation of the spectrometer electronics. This test requires cable connections.

Use two BNC-to-BNC cables to connect the Laser output to the Sync input and the Internal Detector output to the Channel B input.



Time-resolved

TRS

This test checks the step-scan time-resolved circuitry in the spectrometer and is available only if your system is equipped with the optional OMNIC SST with Time-Resolved Experiments software

Notice

If you are not planning to run a TRS experiment, disconnect the data acquisition card cables from the spectrometer when you finish running the TRS tests. Never leave the spectrometer connected to the data acquisition card when you are not running TRS experiments or tests. It could affect your data. ▲

You do not need to set any TRS setup parameters before running this test. Your parameters will be restored when the test is completed. The results will be reported as the signal-to-noise ratio and will indicate whether the spectrometer passed or failed.

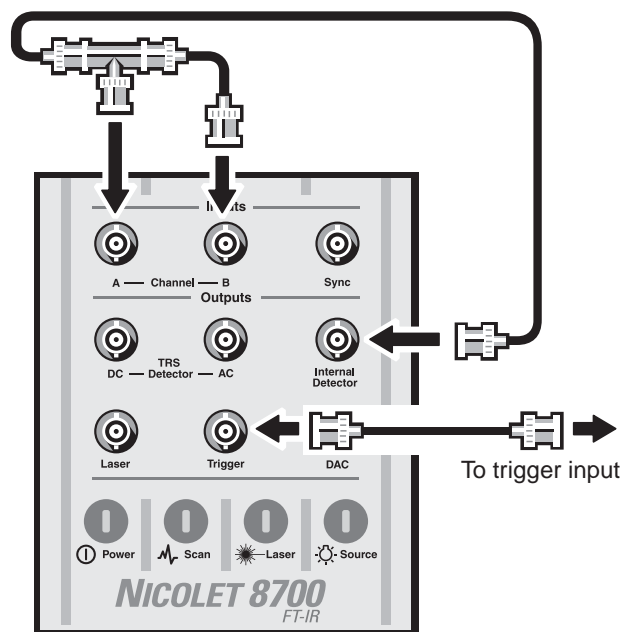
You must install cables before selecting this test. You may also need a data acquisition card installed in your computer. During the test, Choose Yes when prompted for information about the background source.

- 1. Install a BNC “T” connector on the Channel A input connector on top of the spectrometer.**
- 2. Install three BNC-to-BNC cables.**

Use one cable to connect the Channel A input and the Internal Detector output on top of the spectrometer.

Use a second cable to connect the Channel A input to the channel 1 input on the data acquisition card (or the Channel B input connector on top of the spectrometer, for internal TRS data collection).

Use a third cable to connect the Trigger output on top of the spectrometer to the trigger input (EXT) on the data acquisition card.



Troubleshooting Software

The OMNIC software automatically and continuously checks the status of your system. If a problem is found, a message automatically appears giving you access to more information. This chapter lists some simple troubleshooting measures you can take to solve software problems with OMNIC. If the action does not solve the problem, call technical support.



In OMNIC Help Topics find “troubleshooting” in the Index and go to “Troubleshooting” for more information.

Problem	Possible Cause	Solution
After data collection, message says sample and background spectra have wrong resolution.	Resolution of current background spectrum does not match resolution selected for sample spectrum collection.	Change Resolution to match background and collect spectrum again. Use Resolution parameter on Collect tab of Experiment Setup dialog box.
Quantify command is dimmed.	No quantitative analysis method is selected.	Select quantitative analysis method using Quant Setup in Analyze menu. Select single spectrum. Select appropriate method for selected spectrum.

Problem	Possible Cause	Solution
<p>You cannot add spectrum to user library.</p>	<p>Resolution of spectrum is lower (higher numerical value) than that of library.</p>	<p>Collect spectrum at same resolution as library (first set Resolution on Bench tab of Experiment Setup dialog box), and then add it to library.</p>
	<p>The spectrum is from a commercial library.</p>	<p>Only spectra you collect can be added to a user library. Commercial libraries cannot be altered and the spectra contained in them cannot be copied to other libraries.</p>
<p>OMNIC needs to be restored after system crash, or message states that OMNIC cannot start or will no longer run.</p>	<p>There is not enough memory.</p>	<p>Make sure OMNIC has enough memory. Quit other programs to free memory for OMNIC.</p>
	<p>There is another system problem.</p>	<p>Restart Windows. Run SCANDISK utility included with your Windows software. Restart OMNIC. If OMNIC does not start, reinstall it.</p>
<p>Experiment provided with OMNIC does not produce good results.</p>	<p>Parameter settings in experiment file have been changed so that experiment is no longer useful.</p>	<p>Restore experiment to its default settings: First open experiment using Experiment Setup and save it using new filename if you do not want to overwrite it. Then open experiment in FACTORY directory whose filename is same as original experiment and save it in Omnic\Param\Factory directory.</p>

Problem	Possible Cause	Solution
Desired experiment does not appear in Experiment drop-down list box.	Experiment was installed with software but has not yet been opened.	If experiment was designed for Smart accessory, install accessory; experiment will be opened automatically and will appear in Experiment drop-down list box. If experiment was not designed for Smart accessory, open it using Experiment Setup; it will be added to list.
Libraries created with previous version of OMNIC are not listed in Library Setup dialog box.	Libraries are not in one of directories listed in dialog box (typically LIBS within OMNIC directory).	Use Add Directory button on Search Libraries tab to add directory

Troubleshooting Hardware

The OMNIC software automatically and continuously checks the status of your system. If a problem is found, a message automatically appears giving you access to more information. This chapter lists some simple troubleshooting measures you can take to solve software problems with OMNIC. If the action does not solve the problem, call technical support.



In OMNIC Help Topics find “troubleshooting” in the Index and go to “Troubleshooting” for more information.

OMNIC continuously monitors the operation and status of your spectrometer and informs you if a problem is found. The Bench Status indicator below the menu bar shows the status of the spectrometer operation. When OMNIC performs a check and detects a problem, the Bench Status indicator is displayed as a yellow circle or a red X along with a message alerting you to the problem.



If the indicator is a yellow circle, a cooled detector in the Nicolet 8700 has become warm. A message appears explaining the problem and allowing you to access information on correcting it.



If the indicator is a red X, the spectrometer has failed a diagnostic test and requires corrective action. A message appears explaining the problem and allowing you to access information on correcting it.

This chapter lists some simple troubleshooting measures you can take to solve problems with the spectrometer. The diagnostics software is described in the “Diagnostics” chapter. If your actions do not solve the problem, call your Nicolet service office.



For more troubleshooting information see the “Troubleshooting” book in Spectrometer Help Topics.

⚠ Warning

Always follow the safety precautions included in this manual and in your *Spectrometer Safety Guide* when performing any of the following troubleshooting procedures. ▲

Problem	Possible Cause	Solution
Status indicators do not light when spectrometer is turned on.	Spectrometer is not plugged in.	Make sure power cord is plugged into spectrometer and working wall outlet.
	Power cord or power supply is defective.	In Spectrometer Help Topics view “Replacing the power supply” in “Replacing parts” to find part number, ordering and installation instructions.
Data are not displayed during collection.	Laser is not functioning.	Hold business card or other small piece of white paper in beam path in sample compartment to check for laser light. Replace laser if necessary. In Spectrometer Help Topics view “Replacing the laser” in “Replacing parts” to find part number, ordering and installation instructions.
	Data cable between spectrometer and computer is not properly connected.	Turn spectrometer power off and check data cable connections. If the cable is damaged, replace it. In Spectrometer Help Topics view “Cables and connectors” in “Ordering parts” to find part number, and ordering information.

Problem	Possible Cause	Solution
Source status indicator is off.	Source is burned out.	In Spectrometer Help Topics view “Replacing your source” in “Replacing parts” to find part number, ordering and installation instructions.
System does not scan.	Laser is flickering.	Hold business card or other small piece of white paper in beam path in sample compartment to see if laser light flickers. If it does, call Thermo Fisher for service.
There is frost on outside of detector.	Insulating vacuum chamber surrounding dewar has begun to leak.	If you suspect your detector has vacuum leak, view “Detector does not stay cooled” in “Troubleshooting” in Spectrometer Help Topics.
Signal intensity is low, there are frequent modulator scan restarts (verified by intermittent flashing of Scan indicator) and spectrometer alignment fails.	Beamsplitter is fogged.	Check laser signals by clicking laser indicator on Diagnostic tab in Experiment Setup dialog box. If you suspect beamsplitter is fogged, call Thermo Fisher for service.
Baseline is not stable.	Purge rate is too high.	Lower purge rate until baseline is stable. In Spectrometer Help Topics view “Setting purge gas controls” in “Installing optional hardware” for recommended settings.

continued...

Problem	Possible Cause	Solution
	Center laser detector is misaligned.	Use diagnostics software to check laser levels for proper balance. If levels are out of tolerance, align spectrometer using Align button on Diagnostic tab in Experiment Setup dialog box. See the instructions in the Maintenance and Service chapter earlier in this manual. If levels remain out of tolerance, call Thermo Fisher for service.
	Desiccant is expired.	Replace desiccant. In Spectrometer Help Topics view “Checking and changing desiccant” in “Maintaining your spectrometer” to find part number, ordering and installation instructions.
	Spectrometer cover was recently opened.	Allow spectrometer to purge for 3 to 5 minutes after cover is closed.
Signal intensity is low in mid-IR range.	Source is glowing unevenly.	Check to see if source element is glowing evenly. If it is not, in Spectrometer Help Topics view “Replacing the source” in “Replacing parts” to find part number, ordering and installation instructions.
System scans but gives very low signal intensity.	Spectrometer is out of alignment.	Align spectrometer using Align button on Diagnostic tab in Experiment Setup dialog box. See the instructions in the Maintenance and Service chapter earlier in this manual.

continued...

Problem	Possible Cause	Solution
	<p>Detector and beamsplitter are not compatible</p>	<p>Make sure that selected detector and beamsplitter are compatible. Change detector or beamsplitter if necessary. In Spectrometer Help Topics view “Replacing the detector” in “Replacing parts” and/or “Changing beamsplitters” in “Setting up experiments” for instructions.</p>
	<p>There is no interferogram.</p>	<p>If Source status indicator is off, click source indicator on Diagnostic tab in Experiment Setup dialog box to check source current and voltage.</p> <p>If Source indicator is on, check interferogram on Bench tab in Experiment Setup dialog box; if interferogram is not present, check beam path and detector.</p>
<p>You encounter problems when selecting external detectors on AEM, GC interface or microscope.</p>	<p>Custom detector is selected on Bench tab of Experiment Setup dialog box.</p>	<p>Set Detector to None on Bench tab of Experiment Setup dialog box.</p>
	<p>Detector cable is loose at accessory connector (on rear of spectrometer or on back wall of sample compartment).</p>	<p>Check and tighten cables.</p>

continued...

Problem	Possible Cause	Solution
	<p>Detector interface cable is loose at accessory connector (on rear of spectrometer or on back wall of sample compartment).</p>	<p>Check and tighten cables.</p>
	<p>Detector interface configuration for detector type and/or detector address incorrectly set.</p>	<p>Change the configuration settings. In SST Help Topics view “Detector Interface” in “Hardware setup > Optional kits” for specific information.</p>
<p>Signal intensity is low, there are frequent modulator scan restarts (verified by intermittent flashing of Scan indicator) and spectrometer alignment fails.</p>	<p>Beamsplitter is fogged</p>	<p>Check laser signals by clicking laser indicator on Diagnostic tab in Experiment Setup dialog box, remove beamsplitter and check beamsplitter center window for fogging (check clear area located in center of substrate). Replace beamsplitter if necessary. In Spectrometer Help Topics view “Changing beamsplitters” in “Setting up experiments” for part number, ordering and installation information.</p>
<p>Laser status indicator is off.</p>	<p>Beamsplitter compartment cover is not fully closed.</p>	<p>Close and latch the beamsplitter compartment cover.</p>
	<p>Laser is burned out.</p>	<p>View “Replacing the laser” in “Replacing parts” in Spectrometer Help Topics to find part number and ordering and installation instructions.</p>

Problem	Possible Cause	Solution
Scan status indicator does not flash (system is not scanning).	Spectrometer is out of alignment.	Align spectrometer using Align button on Diagnostic tab in Experiment Setup dialog box. See the instructions in the Maintenance and Service chapter earlier in this manual.
	After 1 hour without data collection activity, interferometer stops scanning and Scan light stays on. This mode is normal.	No action is required. Any data collection activity will cause interferometer to begin scanning.
	Beamsplitter is not properly seated.	Check beamsplitter and reposition it if necessary. In Spectrometer Help Topics view “Changing beamsplitters” in “Setting up experiments” for instructions.
Scan status indicator does not flash (system is not scanning).	Beamsplitter compartment cover is ajar.	Close cover and latch it. In Spectrometer Help Topics view “Changing beamsplitters” in “Setting up experiments” for instructions.
	Electronic miscue has occurred.	Cycle power to the spectrometer.
	Component has failed.	Contact Thermo Fisher for service

Problem	Possible Cause	Solution
<p>Error message appears when you try to scan.</p>	<p>Light source is not working.</p>	<p>Check Source status indicator. If light is out, replace source. In Spectrometer Help Topics view “Replacing the source” in “Replacing parts” to find part number, ordering and installation instructions.</p>
	<p>Detector is not cooled.</p>	<p>Cool the detector. In Spectrometer Help Topics view “Cooling a detector” in “Setting up experiments” for instructions</p>
	<p>Interferogram peak is not located at 1024 ± 16 data points in the live display on the Bench tab in Experiment Setup dialog box.</p>	<p>Align spectrometer. See the instructions in the Maintenance and Service chapter earlier in this manual. If the interferogram peak still is not located correctly, call Thermo Fisher for service.</p>
	<p>Beam path is blocked.</p>	<p>Hold business card or other small piece of white paper in beam path in sample compartment to check for laser light. If no laser light is visible, beam path may be blocked. Remove obstruction.</p>

Problem	Possible Cause	Solution
Error message appears when you try to scan.	Data cable between spectrometer and computer is not properly connected.	Turn off spectrometer power and check data cable connections. If the connections are loose, seat the connector firmly and secure the connection with the strain relief. If the cable is damaged, replace it. In Spectrometer Help Topics, find “Cables and connectors” in “Ordering parts” for part number and ordering information.
	Detector, source, and beamsplitter are not compatible	In Spectrometer Help Topics, see “Selecting a beamsplitter, detector, and source” in “Setting up experiments” for a listing of compatible combinations. Change detector, beamsplitter, or source, as necessary.

Troubleshooting Applications

If you have turned on OMNIC's spectral quality checks feature, the software automatically checks the status of collected interferograms, and background and sample spectra.



When OMNIC performs a check and detects a problem with data collection or spectra, the Collect Status indicator is displayed as a yellow circle or a red X. You can click the indicator (or click the View Collect Status button at the end of data collection) to see a summary of data collection problems encountered.

This chapter lists some simple troubleshooting measures you can take to solve data collection problems with the spectrometer. If the action does not solve the problem, contact technical support.



In OMNIC Help Topics find “troubleshooting” in the Index and go to “Troubleshooting” for more information.

Problem	Possible Cause	Solution
Spectrum contains derivative-shaped peaks.	Sample in diffuse reflection experiment also has specular reflection component.	Correct spectrum by using Other Corrections in Process menu. (Select Kramers-Kronig.)
	Infrared beam was reflected from (instead of penetrating) flat, shiny sample measured using specular reflection accessory.	Try using less reflective sample.

Problem	Possible Cause	Solution
Spectrum contains totally absorbing peaks.	Sample in transmission experiment is too thick.	Use thinner sample.
Spectrum contains carbon dioxide peaks.	Spectrometer is not adequately purged.	Make sure you are using correct purge gas and that purge flow rate is adequate. See “Checking the purge” in the Before You Collect Spectra chapter earlier in this manual. Allow system three to five minutes to reestablish purge before collecting spectrum.
Spectrum contains water peaks.	Spectrometer is not adequately purged.	Make sure you are using correct purge gas and that purge flow rate is adequate. See “Checking the purge” in the Before You Collect Spectra chapter earlier in this manual. Allow system three to five minutes to reestablish purge before collecting spectrum.
	Desiccant is expired.	Check desiccant and replace it if needed. In Spectrometer Help Topics view “Checking and changing desiccant” in “Maintaining your spectrometer” to find part number, ordering and installation instructions.
There are no peaks in spectrum.	There is no sample in infrared beam path.	Check sample compartment or accessory to make sure sample is properly positioned in beam path.

continued...

Problem	Possible Cause	Solution
	Sampling cup in diffuse reflection experiment is not in place or is tilted.	Make sure cup is properly positioned in diffuse reflection accessory.
	Infrared microscope is in its viewing mode.	Put microscope in infrared mode and collect spectrum again.
	Sample film in attenuated total reflection (ATR) experiment is being held against ATR crystal with uneven pressure or has poor contact with crystal.	Make sure sample is held evenly and has good contact with crystal.
Spectrum contains fringes or channeling.	Sample has parallel, highly reflective sides that cause infrared beam to bounce within sample when it is placed perpendicular to beam	<p>Create new film using matte press.</p> <p>Try roughening film surface slightly with silicon carbide paper or other suitable abrasive.</p> <p>Rotate sample so that infrared beam passes through sample at Brewster's angle. (Do not use this method if you are performing quantitative analysis of sample.)</p>
Baseline of spectrum is not flat.	KBr pellet was made with coarsely ground KBr powder, or KBr pellet was improperly pressed.	Be sure to press pellet properly.

continued...

Problem	Possible Cause	Solution
	Background spectrum for cast film was collected with empty sample	Remove sample holder and collect background again.
	Spectrometer is not properly aligned, causing sloped baseline.	Use Align button on Diagnostic tab in Experiment Setup dialog box to align spectrometer. See the instructions in the Maintenance and Service chapter earlier in this manual.
	Spectrometer has not been on long enough to reach thermal equilibrium.	For best results allow spectrometer at least one hour to stabilize after turning it on.
	Spectrometer is not properly purged.	Make sure you are using correct purge gas and that purge flow rate is adequate. See “Checking the purge” in the Before You Collect Spectra chapter earlier in this manual. Allow system three to five minutes to reestablish purge before collecting spectrum.
Spectrum is too noisy.	Detector is saturated.	Add bandwidth-limiting filters or energy screens to reduce signal strength.
	There were too few scans.	Increase number of scans on Collect tab in Experiment Setup dialog box.
	Resolution was too high.	Reduce resolution on Collect tab in Experiment Setup dialog box.

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