

NETXUS
F T - I R S P E C T R O M E T E R S TM

870 User's Guide

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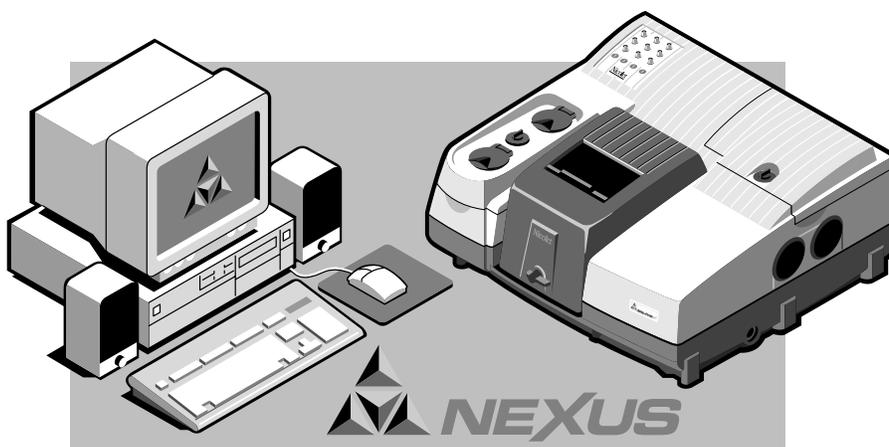
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Welcome

Congratulations on your purchase of a Nexus™ 870 spectrometer from Nicolet! The spectrometer lets you collect spectra in the mid-IR, far-IR and near-IR spectral ranges. The 870 has all of the features of the other Nexus spectrometers, plus step-scan, dual channel collection and other advanced features. The system integrates advanced hardware features with the power and flexibility of Nicolet's OMNIC® software*.



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

* Some dedicated systems use other Nicolet software packages.

⚠ Warning

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

The Nexus 870 has these advanced capabilities:

- Step-scan data collection using either amplitude or phase modulation.
- Slow-scan linear data collection.
- Dual-channel linear scan PEM (photoelastic modulation) data collection.
- Optional TRS (time-resolved step-scan) data collection.
- SMM (synchronous multiple modulation) data collection.

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



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

You can also read the “Before You Collect Spectra” and “Your First Experiment” chapters to learn how to start the system and collect and work with spectra.

See “Where to find the information you need” later in this chapter for a description of the on-line documentation provided with the system and for help finding the answers to your questions.

You can replace key parts of the spectrometer, such as the laser and light source. Installation instructions are available on-line. See “Where to find the information you need” for details.

Instructions for most accessories are included with the particular accessory. Additional information on connecting accessories is included in this manual.

You can contact Nicolet at the numbers below. Outside the U.S.A. call your local sales or service representative. Telephone numbers for all Nicolet Customer Support offices are provided with your system.

- Telephone (U.S.A.): 1-800-NICOLET (1-800-642-6538)
- Fax: 1-608-273-5045
- World Wide Web: <http://www.nicolet.com>
- E-mail: nicinfo@nicolet.com

Conventions

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. To access a tutorial, click the Help menu in OMNIC.



This symbol tells you that you can find more information in the on-line OMNIC Help or SST Help systems. Choose OMNIC Help Topics from the Help menu, or choose SST Help Topics from the SST menu.



This symbol tells you that you can find more information in this manual.

Note

Messages like this contain helpful supplementary information about a procedure or technique. ▲

▲ Caution

Follow the instructions given in Cautions to avoid damaging the spectrometer or losing data. ▲

▲ Warning

Always heed the Warnings that appear in this manual to avoid being injured while using the spectrometer. ▲

▲ Danger

Follow the instructions labeled Danger to avoid serious injury or loss of life while using the spectrometer. ▲

System requirements

For optimum performance we recommend that your system have, at a minimum, the following items:

- Intel® Pentium® processor with 166 MHz or greater clock speed.
- At least 64 megabytes of random access memory (RAM).
- The ability to display 16-bit color images.
- Hard disk size of at least 1.0 gigabyte.
- Quad speed CD-ROM drive.
- A 1.44-megabyte floppy disk drive for 3.5-inch floppy disks.
- A 15-inch SVGA monitor with 800 by 600 resolution.
- A keyboard and serial or bus mouse or PS/2®-style mouse.
- 16-bit Sound Blaster compatibility.
- Two serial ports.
- Two open PCI slots.
- One open ISA slot.
- Windows® 98 or Windows NT 4.0 or greater.

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 next chapter for information on starting OMNIC.

The **tutorials** teach you how to do these things:

- Use OMNIC features to collect, display and process spectra.
- Set up your spectrometer for a variety of experiments. You can learn how to change sources, beamsplitters and detectors; install optical filters and screens; and change the sample compartment baseplate.
- Install optional hardware.
- Check and change the desiccant, and purge line filters.
- Change replaceable parts.
- Get part number and ordering information.

Note You must have the Spectrometer Tutorials CD in the computer’s CD-ROM drive to use the “Spectrometer Tour” tutorial or view any videotaped parts replacement procedures in the “Spectrometer Help Topics” tutorial. ▲

You can also find part numbers and hardware setup and replacement procedures with the computer not connected to the spectrometer. Insert the Spectrometer Tutorials CD into the computer’s CD-ROM drive and double-click the icon for the P870_ENU.HLP program.

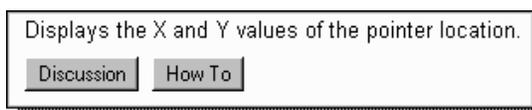
To use a tutorial, choose it from the Help menu or point to Getting Started, Learning OMNIC or Sampling Techniques in the menu and then choose the desired tutorial from the list that appears. You can also start tutorials from within other parts of the on-line documentation provided with OMNIC.

SST Help Topics in the SST menu provides complete information about setting up hardware and software for SST™ experiments.

The **Library Creation Wizard** prompts you, step by step, through creating a user library of spectra.

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

- You can see information about a particular feature in OMNIC (such as a parameter in a dialog box) by clicking the item using the right mouse button. A brief description of the item appears, and in most cases one or more buttons that you can click to display more detailed information. Here is an example:

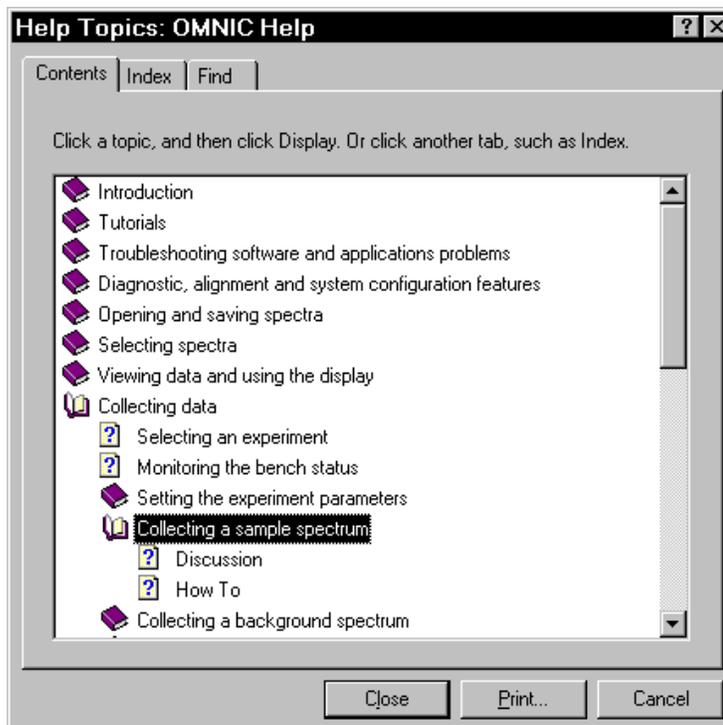


Click the Discussion button to display a complete discussion of the item (or the dialog box or window that contains the feature). Click the How To button to display a step-by-step procedure for using the item (or the dialog box or window that contains the item).

- You can press the F1 function key to see a discussion topic for the currently displayed or selected feature, 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).
- To see the Contents of the OMNIC Help system, choose OMNIC Help Topics from the Help menu.

Here is an example of the Contents tab showing the contents of some of the books in the system:





Before You Collect Spectra

It's easy to collect spectra with your spectrometer. By leaving the system turned on at all times—with the needed components already installed—you can keep it ready to use with a minimum of preparation. Keeping the system on also improves its stability and gives you more consistent results.

All the things you need to check before collecting spectra are listed below; each of these items is discussed in a section of this chapter. By the time you have run through these items once or twice in the course of your work, you will know how to check the system and start collecting spectra quickly.

- Check the purge or desiccant.
- Make sure the system components are on.
- Cool the detector (if you are using an MCT, InSb or other detector that requires cooling with liquid nitrogen).
- Start OMNIC and select an experiment.

Checking the purge

Skip this section if you purchased the “Sealed and Desiccated” option.

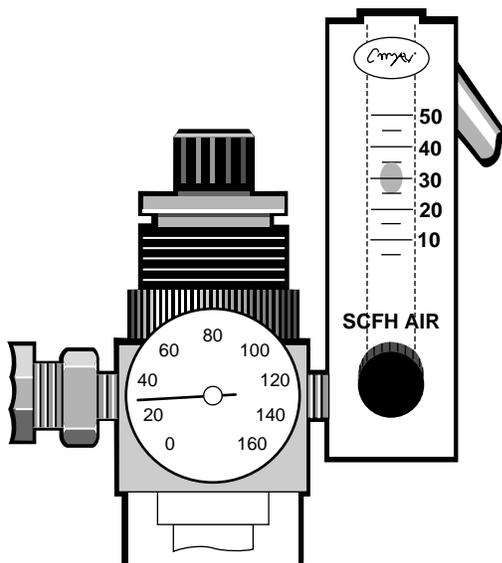
If your spectrometer is purged but you don't have the Smart Purge option, make sure the pressure regulator is set between 20 and 40 pounds per square inch (psi) and the flowmeter reads approximately 30 standard cubic feet per hour (scfh). The settings for Smart Purge are given in the next section; read 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 “Maintaining your spectrometer” for information on how to install the purge equipment, set the controls for the first time, and inspect and clean the purge filter. In the Spectrometer Tour (available through Getting Started) view “Sample compartment” for information on using Smart Purge.

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. See the following table for details.

<i>Flow Rate*</i>	<i>Tank Required?</i>	<i>Comments</i>
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 Nicolet. 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.”

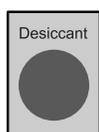
Checking the desiccant



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 bags.

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.**



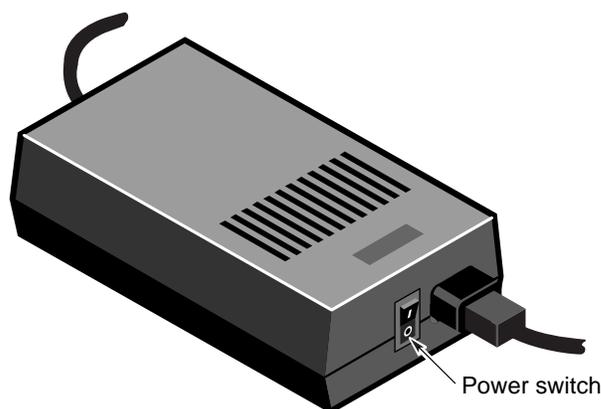
In the Spectrometer Tour (available through Getting Started) view “Connecting to AC power” in the “Powering up” unit for information on connecting the power supply.

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

This includes accessories such as a gas chromatograph, a GC interface 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.

Reverse the order given in the preceding procedure when you turn off system components:

1. Turn off the computer.
2. Turn off the printer.
3. Turn off the spectrometer.
4. Turn off the accessories.

Cooling the detector



Some detectors, such as an MCT or InSb detector, require cooling with liquid nitrogen. 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. ▲

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.

Starting OMNIC

Follow these steps to start OMNIC:

- 1. Start the Windows software.**
- 2. Double-click the OMNIC E.S.P. shortcut.**

The shortcut is on
the Windows desktop.



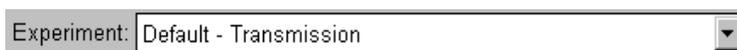
OMNIC E.S.P.

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

The OMNIC window appears. This window is described in the next chapter.

Selecting an experiment

By selecting an experiment from the Experiment drop-down list box below the OMNIC menu bar, you can quickly set the software parameters for the type of data collection you want to perform.



A number of experiments are provided with OMNIC, and you can create and save your own. If you install a Smart Accessory™, the correct experiment is selected automatically (or a list of appropriate experiments is made available for your selection).

In the tutorial in the next chapter the provided Default - Transmission (or Transmission E.S.P.) experiment is used. You will probably find that this experiment is suitable for most of your applications.

If you want to check or change the parameters after selecting an experiment, use Experiment Setup in the Collect menu.

You are now ready to collect spectra.



To learn more about experiments, see “Opening an experiment” in the “Preparing the software” unit of Collecting a Spectrum (available through Learning OMNIC). If you need to install or change a source, beamsplitter or detector for your experiment, follow the instructions in “Setting up experiments” in Spectrometer Help Topics.

Note

The most commonly used hardware configuration for mid-IR experiments includes a KBr beamsplitter, an Ever-Glo™ (mid-IR to far-IR) source and a DTGS detector. You may need to change the settings of the example experiment if your hardware configuration is different. ▲



If you have not used the system before, you can learn how to perform an experiment by viewing Collecting a Spectrum (available through Learning OMNIC) or by using the tutorial in the next chapter of this manual.



Your First Experiment

This chapter will get you started collecting spectra with your spectrometer and working with the data using OMNIC. You will learn how to do the following things:

- Open a configuration.
- Select an experiment and check the parameters.
- Install a sample and collect a sample spectrum.
- Save the spectrum.
- Convert the spectrum to other units.
- Label a peak in the spectrum.
- Verify the composition of the sample by comparing the spectrum with spectra in a QC library.
- Create and print a report containing the spectrum.
- Add the spectrum to a user library.
- Create a user library.



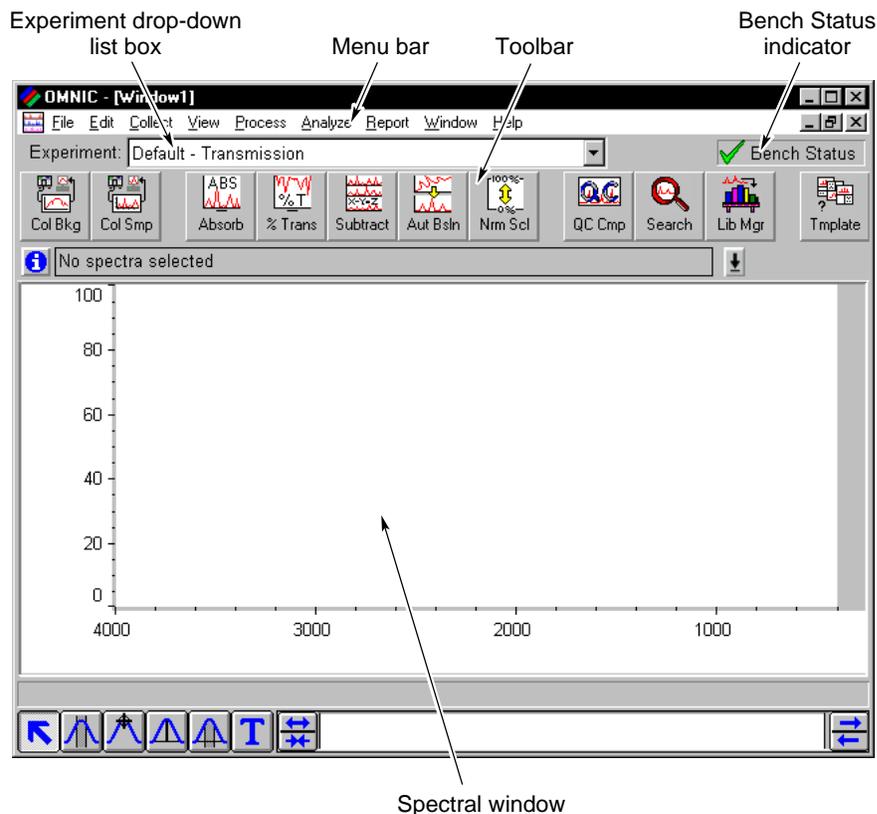
You can learn all these things and more by running the on-line tutorials provided with OMNIC. Start with the Spectrometer Tour and Getting Started With OMNIC (available through Getting Started).

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 on using that software. If you need information on using the spectrometer, see the chapters that follow this one. ▲

The OMNIC window

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



Spectral window

Within the OMNIC window is a spectral window, which you can use to display and manipulate spectra. When a spectrum is displayed in a spectral window, you can use OMNIC commands to perform operations on it. For example, you can change the spectrum's format or search it against a spectral library to identify it.

Menu bar

Below the title bar is the menu bar, which contains all of the OMNIC menu names. The menus are arranged in an order that you'll find convenient as you use the software. All of the menu commands are explained in detail in the on-line tutorials or the OMNIC Help system.

Experiment drop-down list box

Below the menu bar is the Experiment drop-down list box. The Experiment drop-down list contains all of the experiment files you have opened, plus the default experiment file and an experiment file for any Smart Accessory 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 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 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.

Note

If you want to view the on-line videos to help troubleshoot a problem, put the Spectrometers Tutorials CD into the computer's CD-ROM drive. ▲

Toolbar

Below the Experiment drop-down list box is the toolbar. Each button in the toolbar represents a menu command, a macro or an external program. To see the name of the command or feature for a button, point to the button and wait a moment. To initiate the command or feature, click the button with the left mouse button.

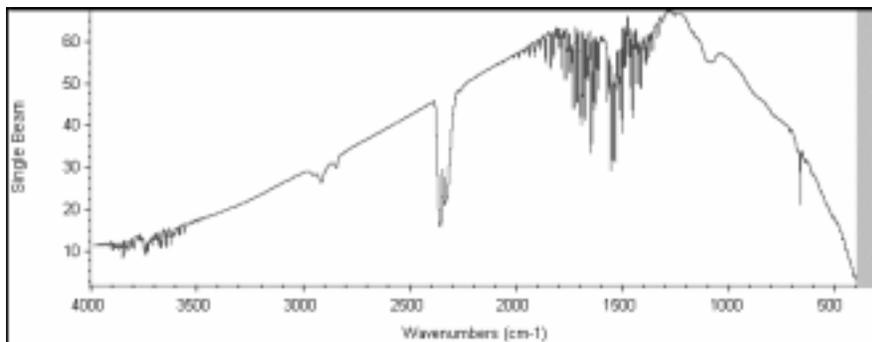


In OMNIC Help Topics find “toolbar” in the Index and go to “Displaying and using a toolbar” for information on using and customizing the toolbar buttons.

Collecting a sample spectrum

A sample spectrum is usually ratioed against a background spectrum. The background spectrum measures the response of the spectrometer without a sample in place. Dividing the sample spectrum by the background—called “ratioing”—removes the effects caused by the instrument and atmospheric conditions so that the peaks in the final spectrum are due solely to the sample.

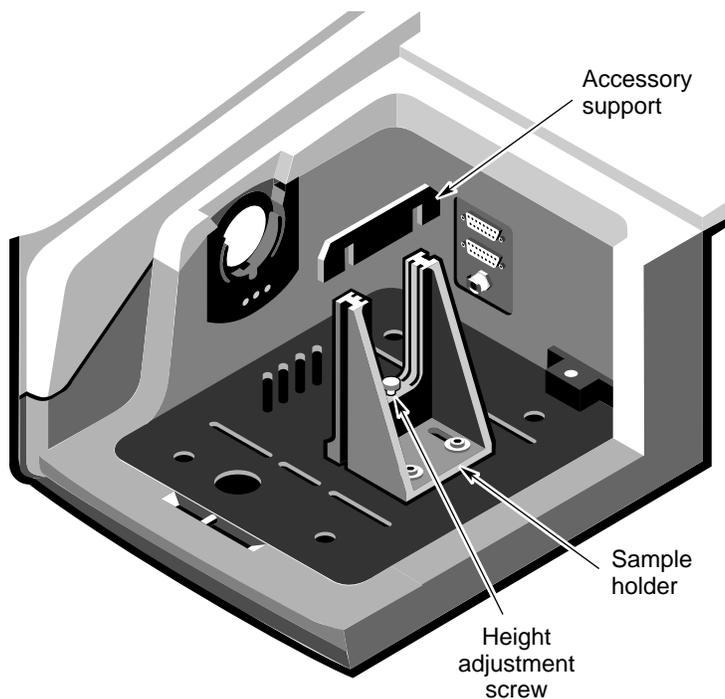
Here is a typical background spectrum:



For most applications you don't need to collect a new background spectrum for each sample spectrum if you haven't changed the software parameters. To obtain good results, however, collect a new background regularly, perhaps once every four hours. (You can obtain the best results by collecting a new background for each sample, but this is seldom necessary.)

Installing the standard sample holder

If the standard sample holder is not already installed, install it now. The following illustration shows the sample holder in place.

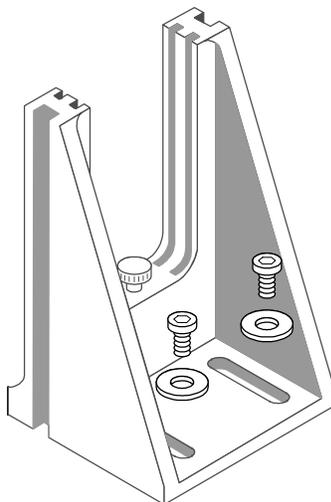


If you are using separate Snap-In™ sample compartment baseplates for different accessories and sample holders, you can quickly switch baseplates to install the sample holder. For information on using Snap-In baseplates, view “Removing the Snap-In baseplate” in “Setting up experiments” in Spectrometer Help Topics.

If your sample holder is mounted on a Smart baseplate, the Transmission E.S.P. experiment is automatically selected when you install the baseplate in the sample compartment.

If your sample holder is not installed on a baseplate, use a flat-blade screwdriver and the slotted screws to attach the holder to a baseplate as shown below. Then install the baseplate in the sample compartment.

If there is a sample in the holder, remove the sample.



To install a sample or filter, slide the sample or filter into one pair of slots. If the accessory support is currently installed in the slot you want to use, remove the support before installing the sample or filter (see the first illustration in this section). Replace the support when you are finished using the slot. *Do not discard the support; it is needed for installing slide-mounted accessories.*

Collecting the sample spectrum

In the data collection procedure that follows, you will collect a background spectrum and then a spectrum of the provided polystyrene sample. Before collecting the spectra, you will open a configuration that sets a number of software options for this procedure.



You can also learn how to collect spectra by viewing [Collecting a Spectrum](#) (available through Learning OMNIC).

Follow these steps:

1. Choose Open Configuration from the File menu.

The Open Configuration dialog box appears listing the available configuration files. Opening one of these files lets you quickly set a number of software options.

2. Select the DEFAULT.CON file and then choose OK.

This file was provided with your OMNIC software for setting the options for this procedure.

3. Select the Default - Transmission experiment (or the Transmission E.S.P. experiment).

Both of these experiments set the parameters correctly for collecting a polystyrene sample spectrum. If either of them is already selected, you do not need to select an experiment. The currently selected experiment is shown in the Experiment box near the top of the OMNIC window.

To select the Default - Transmission (or Transmission E.S.P.) experiment, first click the arrow button at the right end of the Experiment drop-down list box. The Default - Transmission (or Transmission E.S.P.) experiment appears in the list.

Select the Default -
Transmission (or Transmission
E.S.P.) experiment by clicking it.

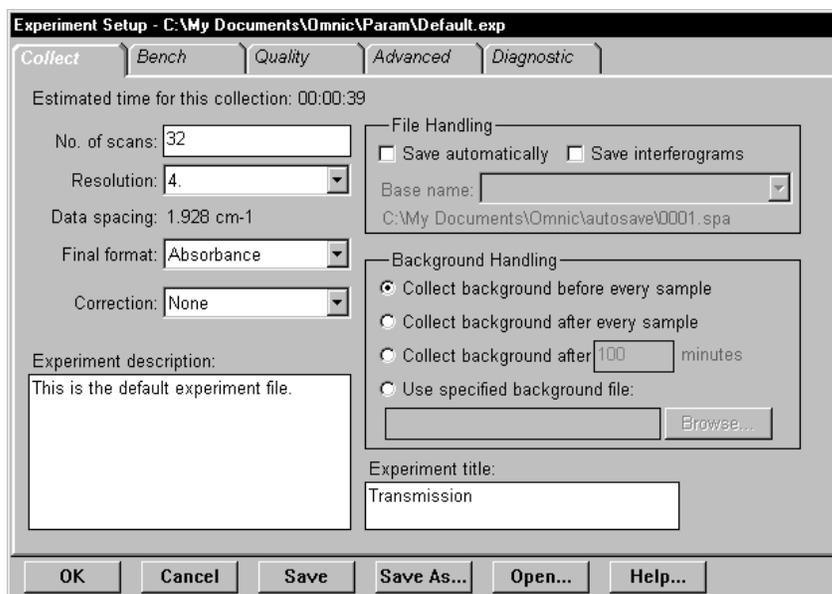


A number of other experiments are provided with OMNIC for performing a wide variety of data collections. You can select these experiments by using the Open button in the Experiment Setup dialog box. After you have selected one of them the first time, the experiment will appear in the Experiment drop-down list for future selection. You can also set up and save your own experiments.

4. Check the settings of the parameters by choosing Experiment Setup from the Collect menu.

This step is normally not necessary, but it's a good way to become familiar with the parameters. The Experiment Setup dialog box appears.

If data collection parameters shown below are not already displayed, click the Collect tab to display them.





The data collection parameters, along with the other experiment parameters, determine how OMNIC collects background and sample spectra. In OMNIC Help Topics find “experiment” in the Index and go to “Using Experiment Setup” for more information.

Notice that the Collect Background Before Every Sample option is selected. This option prompts you to collect a background spectrum before you collect a sample spectrum.

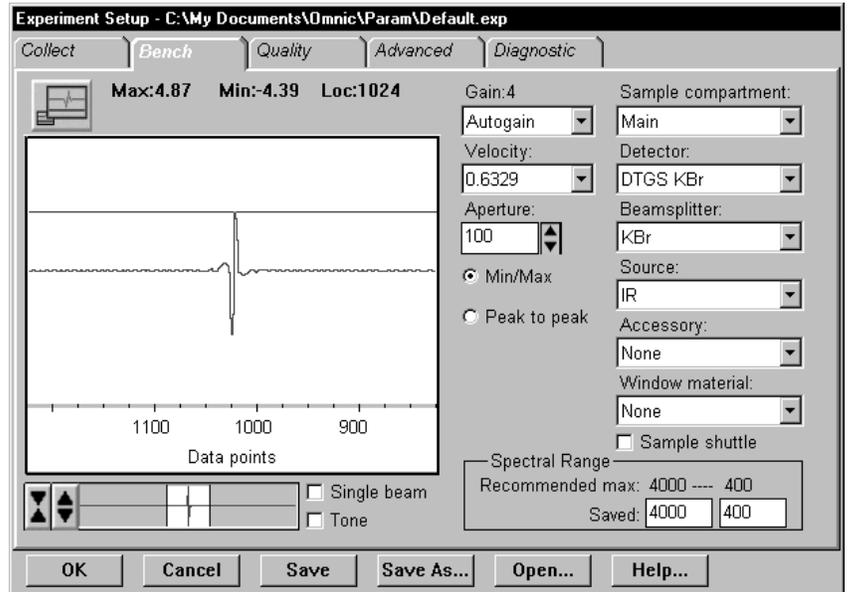
The File Handling box contains options for saving data automatically. When Save Automatically is on, OMNIC saves collected spectra immediately after collection, naming the files using the base name specified in the Base Name box plus a sequence number with up to four digits, followed by an extension such as .SPA for spectra. The files are saved using the path shown below the base name.

If Save Interferograms is on, the interferograms for your spectra are saved when you save the spectra. Interferograms are the raw spectral data. Saving them allows you to reprocess a spectrum later in case you want to restore it after performing corrections or other operations on it.



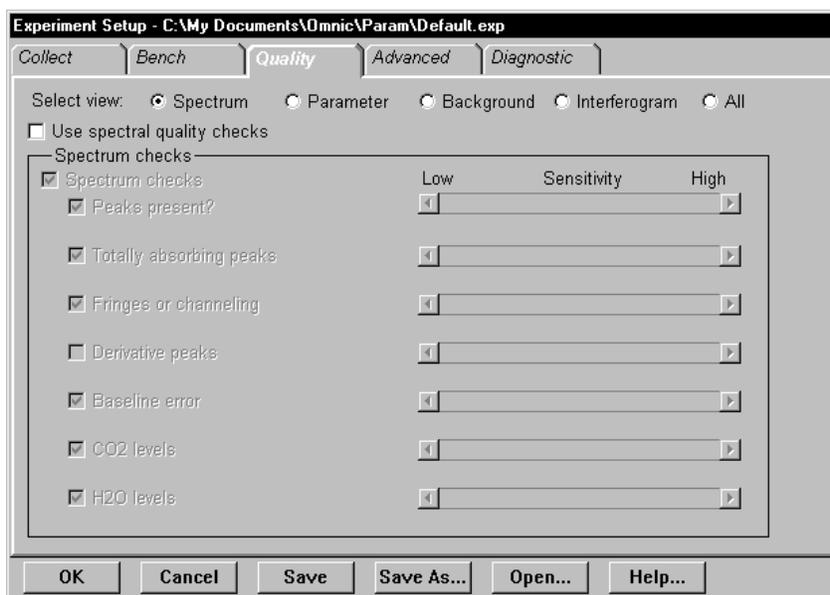
Leave the options in the File Handling box as they are for this procedure. In OMNIC Help Topics find “file” in the Index and go to “File handling” if you want more information on the File Handling options.

Click the Bench tab to display the spectrometer parameters.



Verify that the Beamsplitter, Detector and Source settings match the components you have installed in your system.

Click the Quality tab to display the spectral quality checks.



The selected checks on this tab are performed automatically during data collection. (In the Default - Transmission experiment the checks are turned off.) If a problem is found by a check, the software informs you and provides information to help you correct the problem. This is explained in more detail later in this procedure.

5. Choose OK to close the Experiment Setup dialog box.

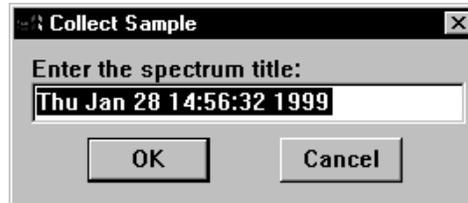
You are now ready to collect a spectrum of the provided polystyrene sample.

6. Click the Collect Sample button in the toolbar.

You can also choose Collect Sample from the Collect menu.

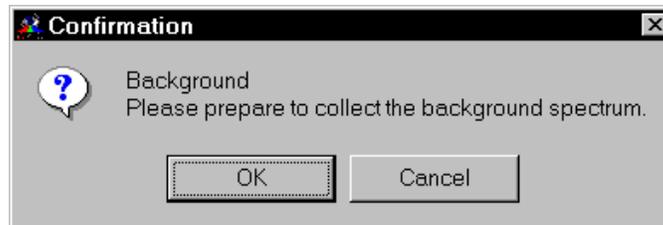


The Collect Sample window appears and then a dialog box showing the default title for the sample spectrum:



7. Type a title in the text box or choose OK to accept the default.

Since the experiment you are using specifies that a background should be collected before every sample, a message appears now asking you to prepare to collect a background spectrum.



This means that you need to remove any sample from the sample holder so that the beam path is clear. When you then collect a background spectrum, the result is a measurement of the response of the spectrometer alone; that is, without absorptions due to a sample.

8. Look through the sliding door to make sure there is no sample in the sample holder and then choose OK to start data collection.

If there is a sample in the sample holder, remove it before choosing OK:

If your spectrometer is purged but does not have the Smart Purge option...

Open the sliding door, remove the sample, close the sliding door and then wait 1 minute before choosing OK.

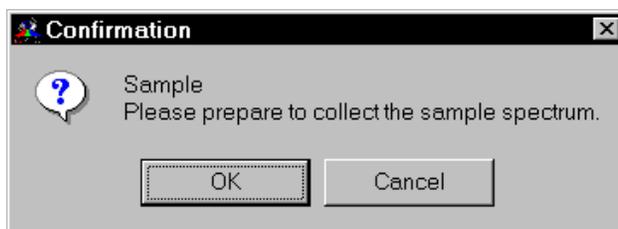
If your spectrometer has the Smart Purge option...

Open the sliding door, remove the sample and then slide the door until it is open about 1 cm. When you hear the purge flow rate return to normal, close the door all the way and choose OK.

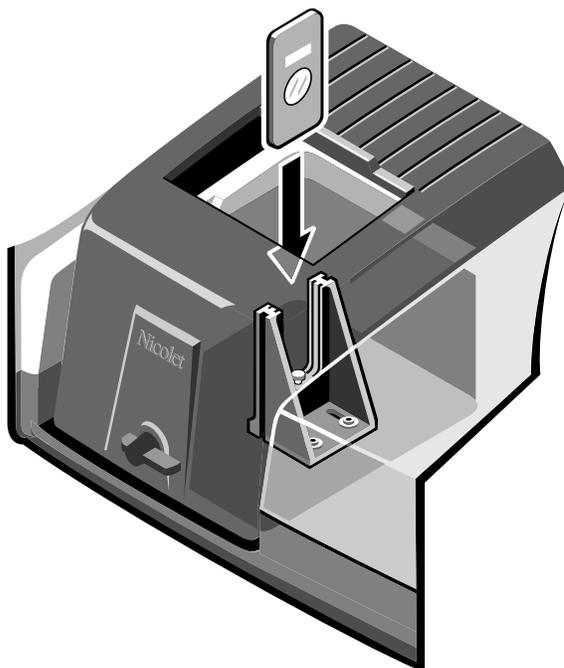
If your spectrometer is sealed and desiccated...

Open the sliding door, remove the sample, close the sliding door and then choose OK.

A background spectrum appears in the Collect Sample window. The spectrum is updated as more data are collected. When all the background data have been collected, a message appears asking you to prepare to collect the sample spectrum:



9. **Install the polystyrene sample through the sliding door, wait if necessary (see the instructions below) and then choose OK.**



If your spectrometer is purged but does not have the Smart Purge option...

Open the sliding door, install the sample, close the sliding door and then wait 1 minute before choosing OK.

If your spectrometer has the Smart Purge option...

Open the sliding door, install the sample and then slide the door until it is open about 1 cm. When you hear the purge flow rate return to normal, close the door all the way and choose OK.

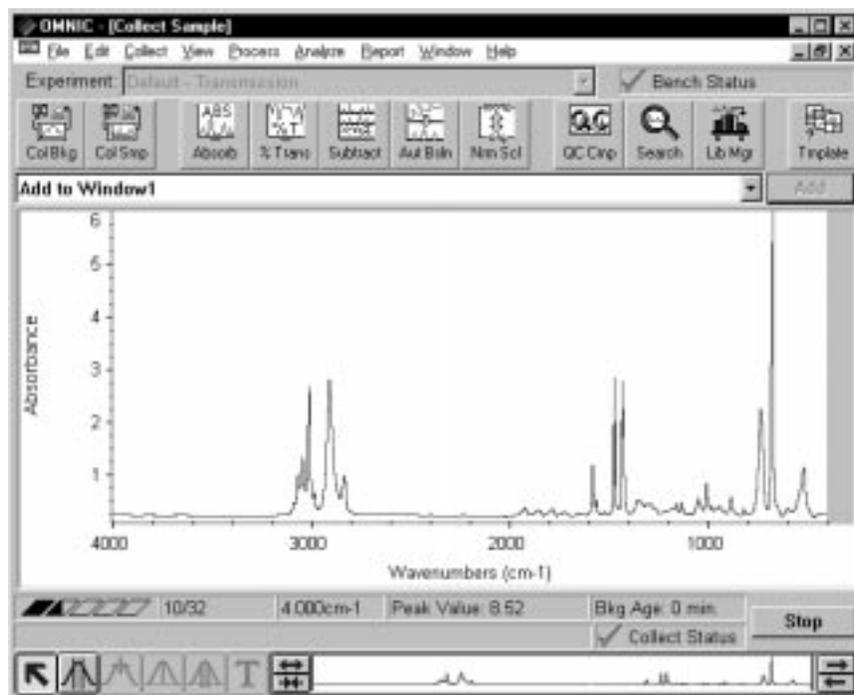
If your spectrometer is sealed and desiccated...

Open the sliding door, install the sample, close the sliding door and then choose OK.



For more information on installing samples, view “Installing Samples” in the Spectrometer Tour (available through Getting Started).

As data are collected, the sample spectrum in the Collect Sample window is updated. Here is the Collect Sample window during sample data collection:



The progress of the collection is indicated visually by the gauge above the tool palette. The number of scans collected so far and the total number of scans for the collection are displayed to the right of the gauge.



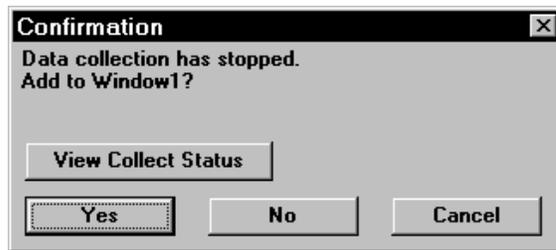
The Collect Status indicator above the view finder shows the status of the collection during and after collection. When the indicator is a green check mark, it shows that the spectrum has passed all of the selected spectral quality checks made so far. After the collection is finished and the indicator 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 any problems that have occurred, click the indicator during or after the collection, or click the View Collect Status button as explained below.

When all the sample data have been collected, the following message appears asking whether to add the spectrum to a spectral window:

Choosing View Collect Status displays the Results window, which shows a summary of problems encountered and other information about the collection.

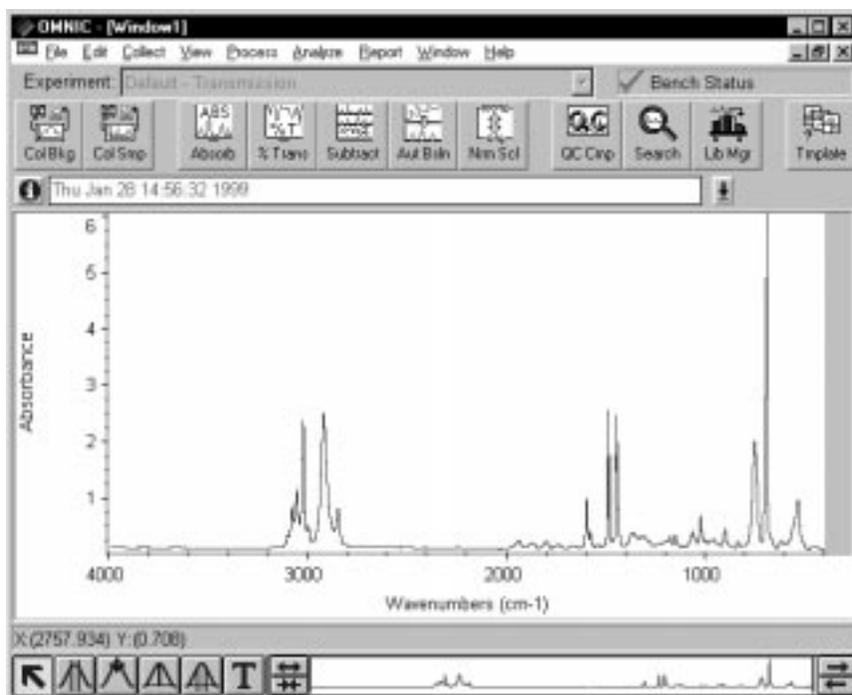


Clicking the View Collect Status button displays the Results window, showing a summary of any problems encountered during data collection and other information about the collection.

10. Choose Yes to add the sample spectrum to the spectral window.

Choosing No ends the procedure without saving the spectrum. Choosing Cancel returns you to the Collect Sample window, allowing you to collect more scans with the More button.

Here is the sample spectrum displayed in the spectral window:



Saving the spectrum

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

Follow these steps to save the polystyrene spectrum you just collected:

1. Select the polystyrene spectrum by clicking it.

2. Choose Save As from the File menu.

The Save As dialog box appears.

3. Type the name POLY.SPA following the directory path in the File Name box.

The text can be either upper or lower case. The default directory path for saving files is determined by the settings on the File tab of the Options dialog box, available through Options in the Edit menu.

4. Choose OK.

If you typed a filename that already exists in the directory, a message appears asking whether to replace the existing file. Choose No and then use a different filename to save the spectrum.

In the next section, you will convert the spectrum to % transmittance and back to absorbance.

Converting the spectrum's units

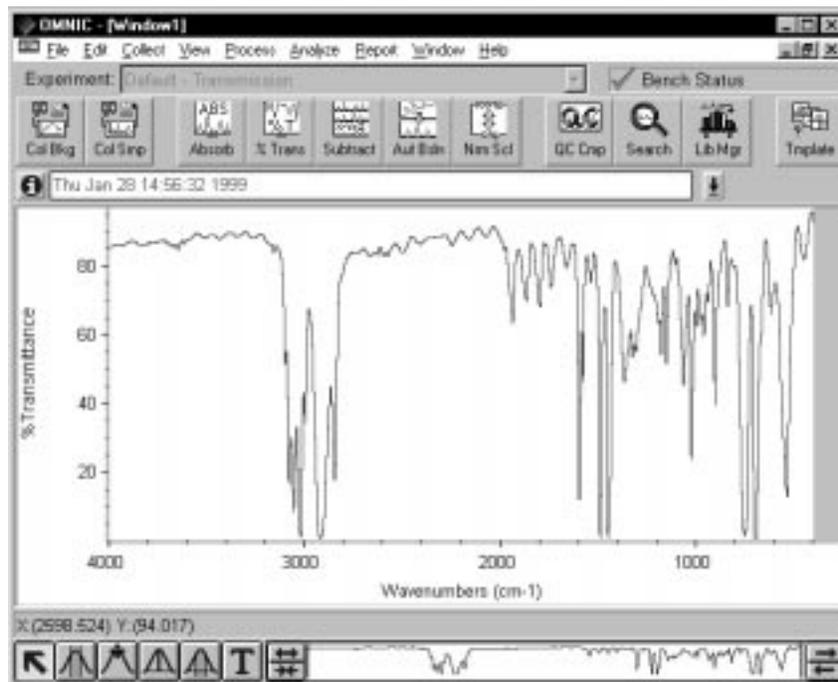
The sample spectrum you collected is in absorbance units. Since many of OMNIC's data manipulation commands work best on spectra in absorbance units, it is often useful to convert a spectrum to absorbance by using the Absorbance command. In this example you will convert the spectrum to % transmittance and then back to absorbance.

1. Select the spectrum by clicking it.
2. Click the % Transmittance button in the toolbar.

You can also choose % Transmittance from the Process menu.



The spectrum is converted to % transmittance units:



Spectrum in % transmittance units



The Process menu allows you to convert spectra to several other units as well. 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.

- 3. Click the Absorbance button in the toolbar to return the spectrum to absorbance units.**

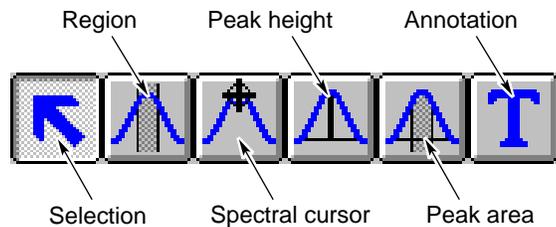
You can also choose Absorbance from the Process menu.



In the next section, you will label a peak in the absorbance spectrum using the annotation tool.

Labeling a peak with the annotation tool

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.



Follow these steps to label a peak in the polystyrene spectrum:

1. Select the annotation tool by clicking it.



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

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; for example, 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 a pane of a spectral window:

X:(3125.792) Y:(1.270)

When the annotation tool is selected and you move the pointer into a pane of a spectral window, the pointer looks like this:

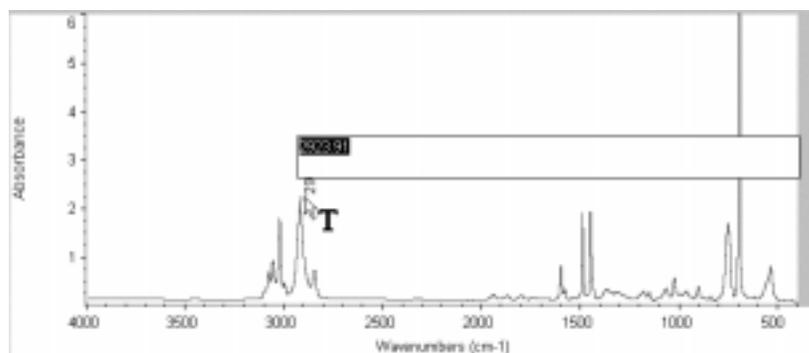


You can label a peak by clicking above it with the annotation tool. This displays the label text above the peak with a line connecting the label to the peak. The text is selected so that you can immediately edit it. When you press Enter, the label appears in its final form.

You can more accurately locate the top of a peak by holding down the Shift key when you click near the peak.

- 2. Label the peak near 2,924 wavenumbers by holding down the Shift key and clicking a little above the peak.**

The label appears:



3. 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 on the annotation tool.

In the next section, you will compare the spectrum with the spectra in a QC library to verify the composition of the sample.

Verifying the composition of the sample

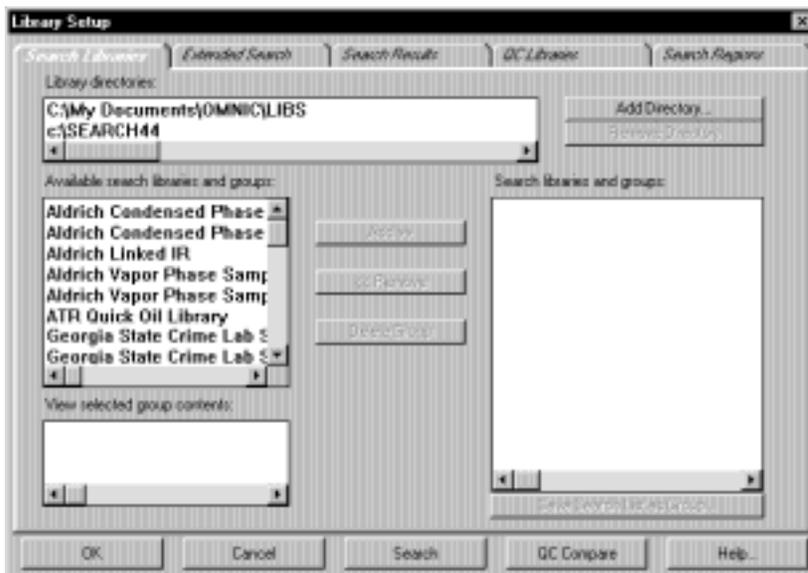
You can verify the composition of your polystyrene sample by automatically comparing the collected spectrum with the spectra in a QC (Quality Control) library. The software compares the sample spectrum with reference spectra in the appropriate category in the library and then tells you whether the sample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



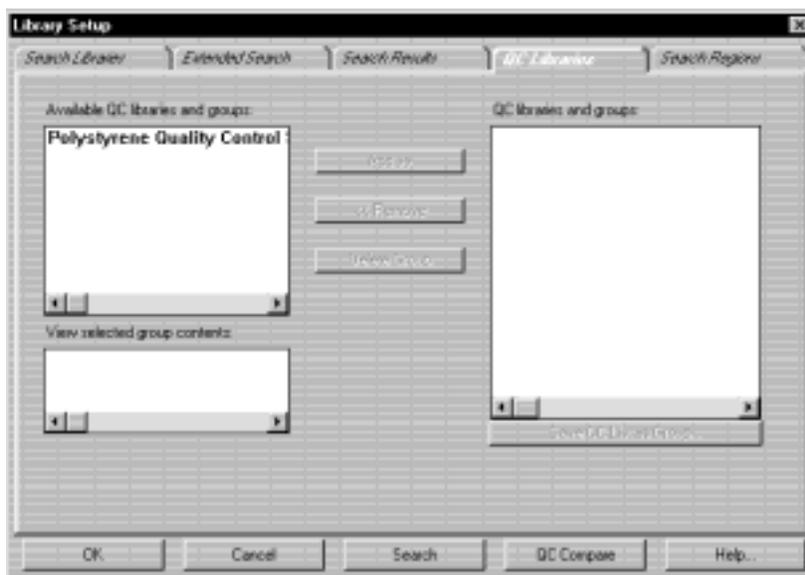
The Library Directories box lists the directories that are currently being used for spectral searches and QC comparisons. All the libraries in the listed directories are available for your QC comparison.

3. Add the LIBS directory (within the OMNIC directory) to the list of directories if it is not already in the list.

This is the directory that 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 Polystyrene Quality Control Sample library 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. In this example the comparison found that the sample spectrum matches the polystyrene spectrum in the library.

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.

Creating and printing a report

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



You can also view Creating Reports (available through Learning OMNIC) to learn how to create and print reports and add them to report notebooks.

1. Choose Template from the Report menu.

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

2. Go to the REPORT directory (within the OMNIC directory) and 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 search results.

When you select the report 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. 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 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.

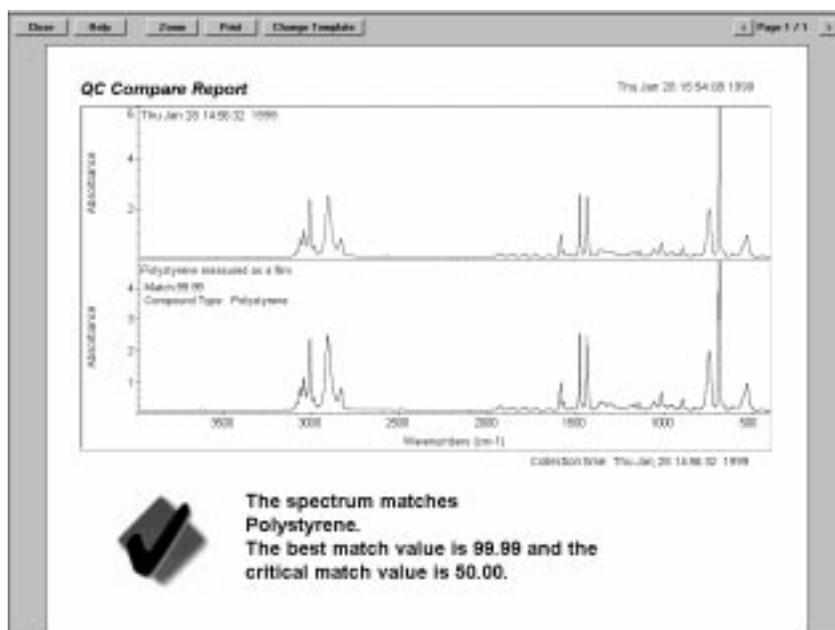


You can create your own report templates by using the Create button, or you can modify one of the existing templates whenever you want to design a new template. Save the template with a new name after you make your changes. In OMNIC Help Topics find “report template, selecting” in the Index and go to “Selecting, editing or creating a report template” for more information on 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. Your report should look similar to this:

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



The preview lets you check the content of the report before printing it.

- 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.**

The report is printed on your system printer.

Adding the spectrum to a user library

You can save your spectrum in a user library even if you have saved it in a spectral data file. This allows you to find the spectrum later by searching for text contained in the information saved with the spectrum. If you add your own reference spectra collected from pure sample materials to a user library, you can also use the library to identify unknown spectra.

Follow these steps to add the polystyrene spectrum to a user library:

- 1. Select the polystyrene spectrum.**
- 2. Choose Add To Library from the Analyze menu.**

The Select Library dialog box appears listing all the user libraries available in the currently specified library directories of the hard disk.

- 3. Select the User Example Library.**

This library has been created for you to use in this example.

4. Choose OK.

The Add To Library dialog box appears showing the name of the library you selected and the index number that has been assigned to the spectrum. The dialog box also contains fields into which you can enter information about the spectrum. The first field already contains the compound name. You can accept or change the text in the fields.

5. When you have finished entering information about the spectrum, choose OK.

You can also add a spectrum to a library by dragging the spectrum or the spectrum's file to the library's book on the Library Names tab of Library Manager.



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

Creating a user library

Creating your own library lets you customize the information in the library depending on your search needs. You can create a search library for identifying unknown spectra, a QC library for verifying the composition of a sample, or a scrapbook library for storing spectra to be retrieved later.

When you create a user library, you determine the kinds of information that will be saved with it. You also set a number of parameters, including the resolution and spectral range of the library and which checks and corrections are performed. The Library Creation Wizard leads you through the steps that are appropriate for the type of library you are creating.

Once a library is created, you can add spectra to it with the Add To Library button (or with Add To Library in the Analyze menu) and use it just as you would a commercial library to identify unknown spectra or verify the composition of a sample. If you create a scrapbook library, you can find spectra in it by searching for text.

In this example you will create a new search library. Follow these steps:

1. Choose Library Manager from the Analyze menu.

Library Manager appears with the Library Names tab in front.

2. Choose Create Library.

The Library Creation Wizard appears.



3. In the Library Creation Wizard, select Search Library, and then enter a name and filename.

The name you enter for the library will appear in the Library Names list when you add a spectrum to a library. You can enter a new filename or accept the default name the Wizard assigns. Click Next to continue.

4. In the next dialog box, enter any comments you wish to record and your name.

The comments you enter will appear in the Comments box on the Library Info tab of Library Manager when you select the library on the Library Names tab. The name you enter will appear in the Created By readout on the Library Info tab when you select the library on the Library Names tab.

5. Add more information about your library.

You can continue entering information about the new library by clicking Next. The Wizard lets you enter information about spectral range, resolution and blanked areas for searching. For this example, click Next in each window.

6. When you have completed entering information, click Finish.

When you click the Finish button, your library is created. You can see the library listed by clicking the Search Libraries book on the Library Names tab of Library Manager.



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



Spectrometer Basics

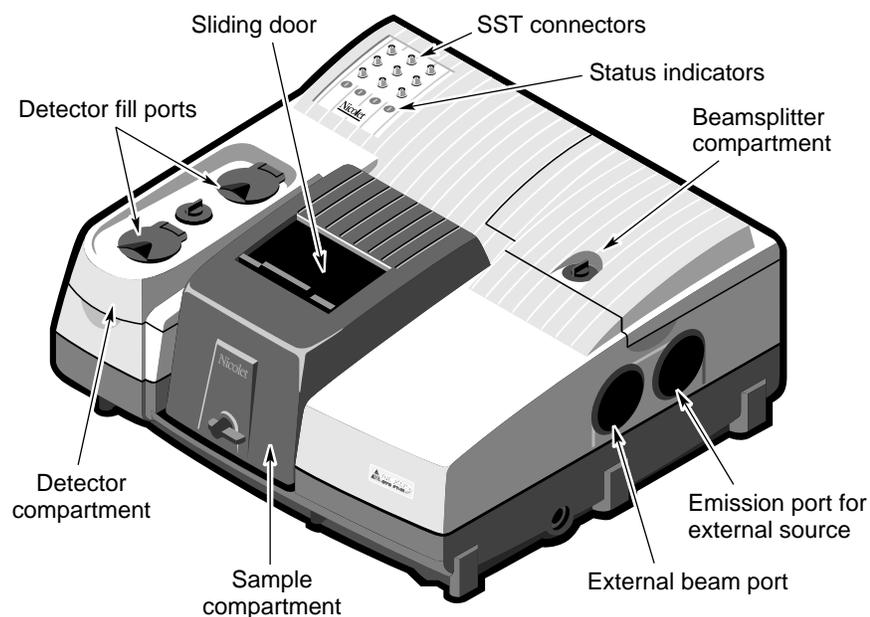
This chapter describes the major components of your Nexus 870 spectrometer, including the light source, beamsplitter and detector. It then explains what you will need to know before collecting data in various spectral ranges.



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 the spectrometer.

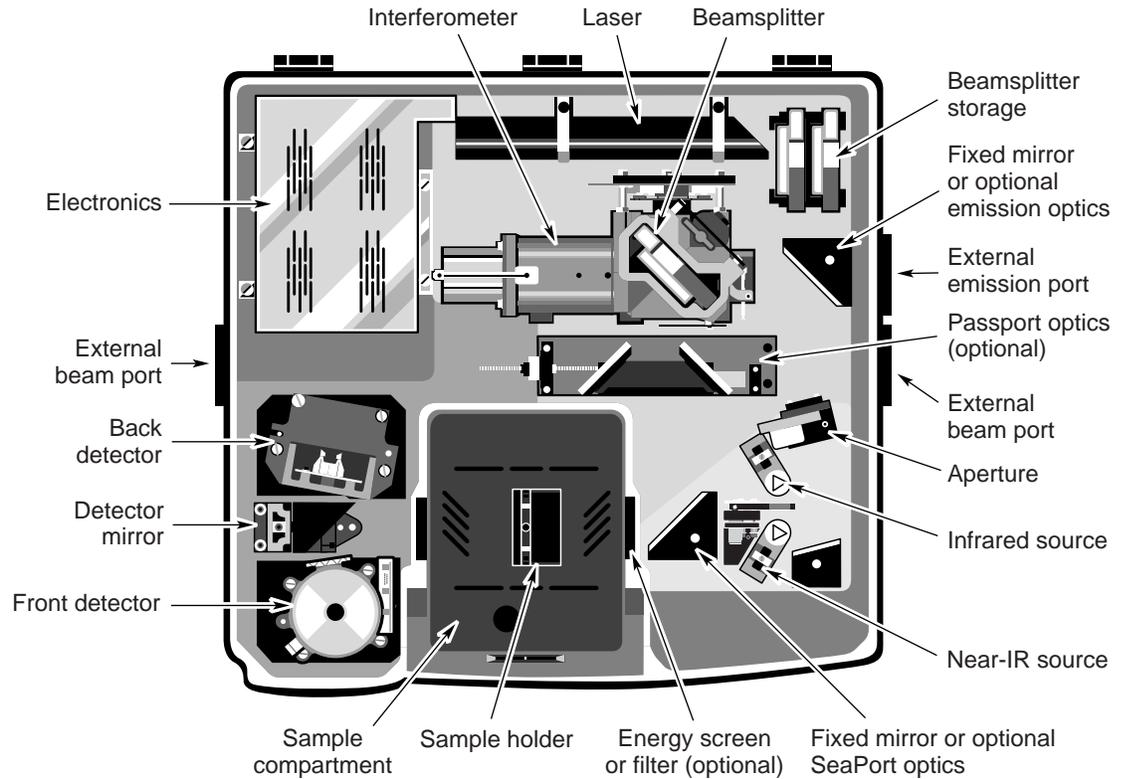




Choose SST Help Topics from the SST menu to find complete information about using the SST connectors.

What's inside?

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

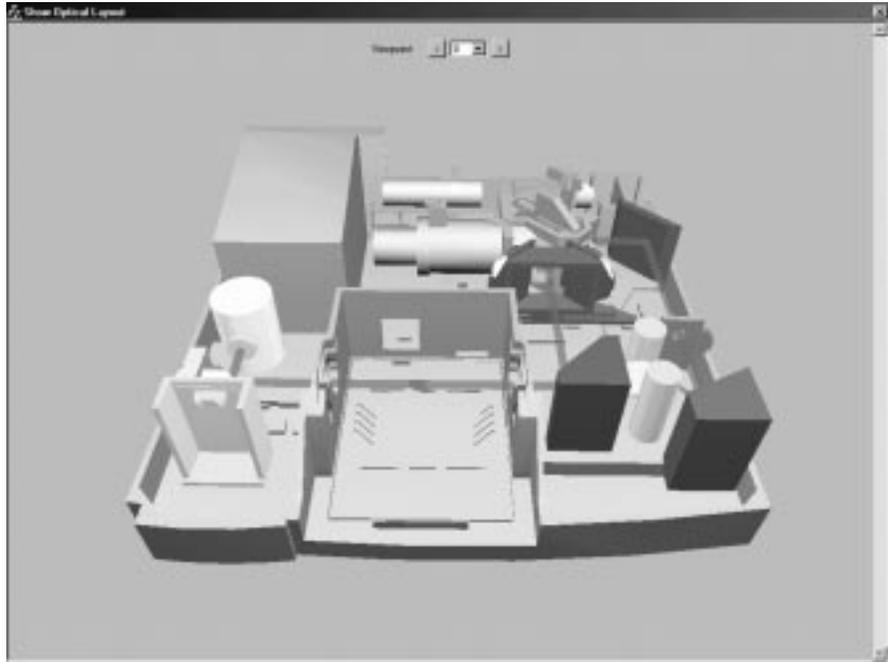


In the Spectrometer Tour (available through Getting Started) view “Inside the spectrometer” for complete descriptions of your spectrometer components.

Viewing the optical layout and beam path in OMNIC

You can view an image of the optical layout showing the current beam path through the system by choosing Show Optical Layout from the Collect menu. Here is an example:

The beam path is indicated by a thick red line.



You can select a different view of the layout from the Viewpoint drop-down list box. If you click the left or right arrow buttons, the view changes in steps.

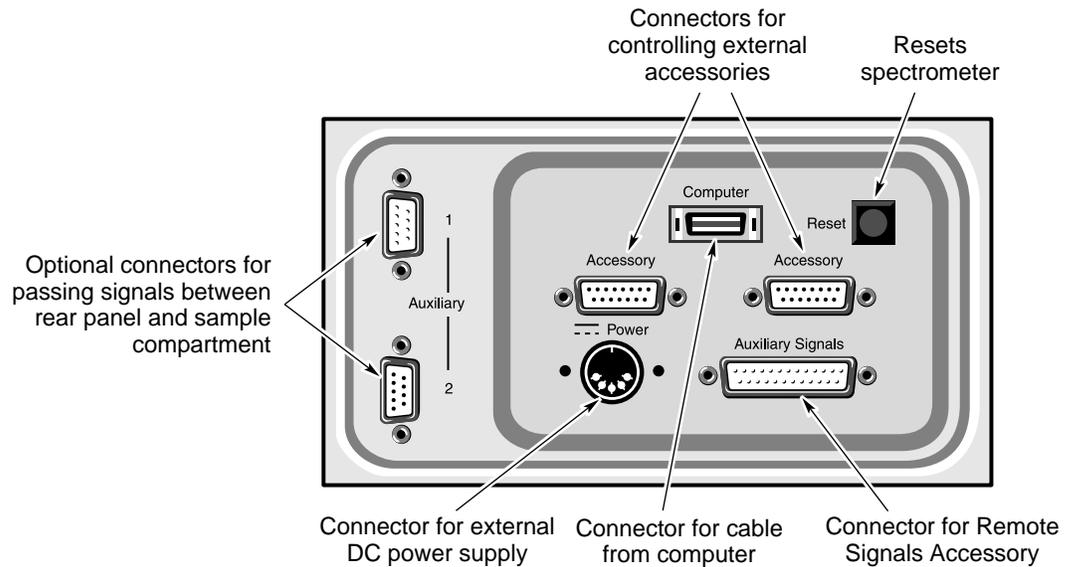
To see what type of detector or source is installed in a location, move the mouse cursor over the image of the component. To select a detector or source, click it. The beam path changes to reflect your selection.



In OMNIC Help Topics find “optical layout” in the Index and go to “Displaying the optical layout” for a complete description of this feature.

What is on the rear panel?

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



Warning

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

Note

Use the Reset button when you are instructed to reset the spectrometer by the troubleshooting procedures found in this manual and elsewhere in the system documentation. ▲



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

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

Turning on the spectrometer power



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 on connecting the power supply.

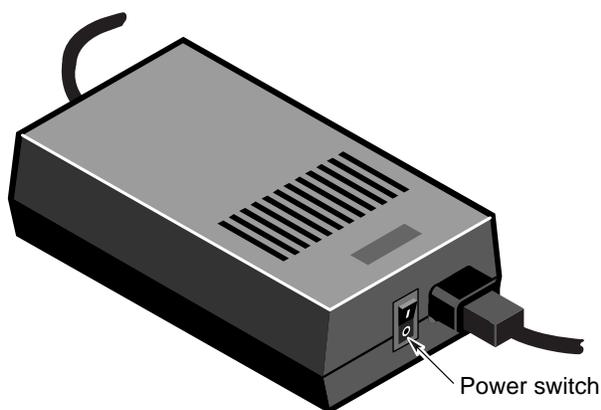
- 2. Turn on any accessories you plan to use.**

This includes accessories such as a gas chromatograph, a GC interface 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.**



To turn the spectrometer off, press the switch to O.

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.

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. ▲

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.

Reverse the order given in the preceding procedure when you turn off system components:

1. Turn off the computer.
2. Turn off the printer.
3. Turn off the spectrometer.
4. Turn off the accessories.



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

Note The system enters a “long-stroke” mode 10 minutes after data collection activity has ceased. This mode continues for 1 hour. After 1 hour, the interferometer stops scanning and the Scan light stays on. Any data collection activity will cause the interferometer to begin scanning. Exiting OMNIC also activates the long-stroke mode. ▲

Note 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, by pressing the Reset button on the rear panel or by turning the spectrometer power off and then on, contact Nicolet at one of the numbers below. Outside the U.S.A. call your local sales or service representative. Telephone numbers for all Nicolet Customer Support offices are provided with your system.

- Telephone (U.S.A.): 1-800-NICOLET (1-800-642-6538)
- Fax: 1-608-273-5045
- World Wide Web: <http://www.nicolet.com>
- E-mail: nicinfo@nicolet.com ▲

Using a light source

The Nexus 870 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.

Warning

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 by a currently installed source, allow enough time for it to cool before handling it. ▲

Nexus 870 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 on using different sources in your spectrometer.

Using beamsplitters and detectors

A number of beamsplitters and detectors are available for use in the Nexus 870. Not all beamsplitters and detectors can be used together. 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.

Selecting the right beamsplitter and detector

There are two considerations when selecting a beamsplitter-detector combination: compatibility and spectral range.

The following table shows which beamsplitter-detector combinations perform best and which are compatible. 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.

DETECTOR	BEAMSPLITTER					
	Near-IR			Mid-IR*		Far-IR
	Quartz	CaF ₂	XT-KBr	KBr	CsI	Solid Substrate
DTGS (KBr window)**	X	OK	Best	Best	OK	X
DTGS (CsI window)	X	X	OK	OK	Best	X
DTGS (PE window)	X	X	X	X	OK	Best
MCT-A	OK	OK	Best	Best	OK	X
MCT-B	OK	OK	Best	Best	OK	X
InSb	OK	Best	OK	X	X	X
PbSe	OK	Best	OK	X	X	X
Si	Best	OK	X	X	X	X
PbS	OK	Best	X	X	X	X
InGaAs	OK	Best	OK	X	X	X

Best = Optimum beamsplitter-detector combination.

OK = Compatible beamsplitter-detector combination.

X = Incompatible beamsplitter-detector combination.

* A ZnSe beamsplitter may also be used as a mid-IR beamsplitter in extremely humid environments.

** Valid for room temperature and thermoelectrically cooled versions.

The next table lists the spectral ranges of compatible beamsplitter-detector combinations.

<i>Light Range</i>	<i>Beamsplitter</i>	<i>Detector</i>	<i>Spectral Range (cm⁻¹)</i>	<i>Source</i>
visible	quartz	PbSe	13,000 - 2,800*	Ever-Glo, white light
		Si [†]	25,000 - 8,600	White light
	CaF ₂	PbSe	13,000 - 2,000*	Ever-Glo, white light
		Si [†]	14,500 - 8,600	White light
near-IR	quartz	MCT-A [‡]	11,700 - 2,800*	Ever-Glo, white light
		MCT-B [‡]	11,700 - 2,800*	Ever-Glo, white light
		InSb ^{‡,§}	11,500 - 2,800*	Ever-Glo, white light
		PbSe	13,000 - 2,800*	Ever-Glo, white light
		PbS TEC (with SabIR)	10,000 - 4,200*	Ever-Glo, white light
		InGaAs	12,000 - 3,800	Ever-Glo, white light
	CaF ₂	MCT-A [‡]	11,700 - 1,200*	Ever-Glo, white light
		MCT-B [‡]	11,700 - 1,200*	Ever-Glo, white light
		InSb ^{‡,§}	11,500 - 1,850*	Ever-Glo, white light
		PbSe	13,000 - 2,000*	Ever-Glo, white light
		PbS TEC (with SabIR)	10,000 - 4,200*	Ever-Glo, white light
		InGaAs	12,000 - 3,800	Ever-Glo, white light
	XT-KBr	MCT-A [‡]	11,000 - 600*	Ever-Glo, white light
		MCT-B [‡]	11,000 - 400*	Ever-Glo, white light
		InSb ^{‡,§}	11,000 - 1,850*	Ever-Glo, white light
		PbSe	11,000 - 2,000*	Ever-Glo, white light
		DTGS-KBr	11,000 - 375*	Ever-Glo, white light
		DTGS TEC	11,000 - 375*	Ever-Glo, white light
		InGaAs	12,000 - 3,800	Ever-Glo, white light

Continued on next page...

<i>Light Range</i>	<i>Beamsplitter</i>	<i>Detector</i>	<i>Spectral Range (cm⁻¹)</i>	<i>Source</i>	
mid-IR	KBr	DTGS-KBr	7,400 - 350	Ever-Glo	
		MCT-A‡	7,400 - 600	Ever-Glo	
		MCT-B‡	7,400 - 400	Ever-Glo	
		DTGS TEC	7,100 - 350	Ever-Glo	
		DTGS-CsI	6,400 - 350	Ever-Glo	
	CsI¶	DTGS-CsI	6,400 - 200	Ever-Glo	
		MCT-A‡	6,400 - 600	Ever-Glo	
		MCT-B‡	6,400 - 400	Ever-Glo	
	ZnSe	DTGS-KBr	4,000 - 650	Ever-Glo	
		MCT-A‡	4,000 - 650	Ever-Glo	
		MCT-B‡	4,000 - 650	Ever-Glo	
		DTGS TEC	4,000 - 650	Ever-Glo	
		DTGS-CsI	4,000 - 650	Ever-Glo	
	far-IR	Solid-Substrate	DTGS-PE	700 - 50	Ever-Glo
			Si bolometer	700 - 20	Ever-Glo

Notes:

- * This spectral range reflects the combination of the ranges of the Ever-Glo and white light sources, as well as the limits of the beamsplitter-detector combination. 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).

Optimizing the performance of your detector

Nexus 870 detectors can be optimized to produce a more linear response and greater photometric accuracy, or to increase the signal-to-noise ratio. You can achieve these improvements in performance by adjusting the amount of infrared energy that reaches the detector.

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.

Look at the low-end region of a single-beam spectrum (below the low-end cutoff); you should see a straight line very near 0. 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.

Note The maximum intensity of a mid-IR single-beam spectrum is typically found near 2,000 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 can result in distorted quantitative data if the background signal is very large.

Check the low-end region of the background and sample interferograms. If you see a substantial difference in their size, photometric accuracy could be a problem.

To solve these problems, Nexus 870 spectrometers allow the following options for modifying the infrared beam:

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



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

In some cases, system performance improves if you use a filter or screen. The filter or screen that you should use for your application depends on the samples being measured and other experimental conditions. Try using various filters or screens to determine which give the best results for your application.

When to use bandwidth-limiting 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.



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

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.

<i>Screen</i>	<i>% Transmitted*</i>	<i>Detectors Typically Used With Screen</i>
none	100	DTGS, MCT-B
A	30	MCT-A
B	10	PbSe, InSb, InGaAs
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 is reduced less than is the signal intensity.



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

What aperture size to use for your detector

The aperture 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 an 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.

DTGS 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 On Nexus spectrometers, the setting of the Aperture parameter determines the *area* of the aperture opening. Doubling the setting approximately doubles the 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 on 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.

<i>Detector</i>	<i>Aperture Setting</i>
DTGS	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 on 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 (using a larger 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 Nicolet Customer Support for assistance. ▲



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

How to improve the 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 on changing the aperture setting.

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 25,000 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.

<i>Spectral Range</i>	<i>Filter or Screen</i>	<i>Aperture</i>	<i>Gain</i>
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 “Installing an optical filter” in the “Setting up experiments” book for instructions on installing filters.

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 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 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.

Note In step-scan experiments, you can use the sample spacing setting alone 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.

<i>Sample Spacing</i>	<i>Nominal Free Spectral Range</i>
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 DTGS/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.

Note If you do not have a 3940 cm^{-1} or 1900 cm^{-1} low-pass filter, you can order one from Nicolet. ▲

Scan velocities

To allow you to collect data faster, OMNIC SST and your Nexus 870 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 moving mirror velocities are available on the Nexus 870, 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.

Sample spacing is set to 4 or 2, or the upper limit of the spectral range is less than or equal to 7899 wavenumbers:

Resolution → Velocity ↓	0.125	0.25	0.5	1.0	2.0	4.0	8.0	16.0	32.0
0.0158 - 5.6961	✓	✓	✓	✓	✓	✓	✓	✓	✓
6.3290	—	—	✓	✓	✓	✓	✓	✓	✓
6.9619	—	—	—	—	✓	✓	✓	✓	✓
7.5948	—	—	✓	✓	✓	✓	✓	✓	✓
8.2277	—	—	—	—	—	✓	✓	✓	✓

Sample spacing is set to 1, or the upper limit of the spectral range is within the range 7900 to 15798 wavenumbers:

Resolution → Velocity ↓	0.125	0.25	0.5	1.0	2.0	4.0	8.0	16.0	32.0
0.0158 - 2.5317	✓	✓	✓	✓	✓	✓	✓	✓	✓
3.1647 - 3.7974	—	—	—	✓	✓	✓	✓	✓	✓
4.4303	—	—	—	—	—	—	✓	✓	✓
4.7468 - 5.6961	—	—	—	—	—	—	—	✓	✓
6.3290	—	—	—	—	—	—	—	—	✓
6.9619 - 8.2277	—	—	—	—	—	—	—	—	—

Sample spacing is set to 0.5, or the upper limit of the spectral range is within the range 15799 to 31596 wavenumbers:

Resolution → Velocity ↓	0.125	0.25	0.5	1.0	2.0	4.0	8.0	16.0	32.0
0.0158 - 1.2659	✓	✓	✓	✓	✓	✓	✓	✓	✓
1.8988	—	—	—	—	—	✓	✓	✓	✓
2.5317	—	—	—	—	—	—	—	—	✓
3.1647 - 8.2277	—	—	—	—	—	—	—	—	—

To specify the 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.

Important 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. ▲

Slow scan 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 DTGS, 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. ▲



View “What is slow scan?” in the “Welcome to Nexus 870!” unit of the Spectrometer Tour (available through Getting Started) for an overview of slow-scan applications.

A note about vibrations

All slow-scan experiments are prone to disruption from vibrations. Should your experiment be disrupted, the Nexus 870 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.

When you finish running slow-scan experiments, use Experiment Setup to change the Velocity setting to 0.6329 cm/s or higher. This is especially important if your next experiment will be a step-scan experiment. The spectrometer cannot automatically shift from slow-scan mode to step-scan mode.



Using the SST Software

The SST menu in OMNIC gives you access to the SST experiments that are available on your system. This chapter provides specific information for using the software to perform each experiment.



View “What is SST?” in the “Welcome to Nexus 870!” unit of the Spectrometer Tour (available through Getting Started) for an overview of the SST software.

Starting the SST software

Follow these steps to start the SST software:

1. Start OMNIC.

Double-click the OMNIC E.S.P. shortcut on the Windows desktop.

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

The OMNIC window appears.

2. Set the experiment parameters.

You can do this in one step by selecting an experiment from the Experiment drop-down list box near the top of the window.

You can also use Experiment Setup in the Collect menu to open an experiment or set the parameters individually. These parameters include File Handling and Background Handling on the Collect tab and Sample Compartment, Detector, Beamsplitter, Source and Aperture on the Bench tab of the Experiment Setup dialog box.

- 3. Click SST in the menu bar to display the SST menu commands.**

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

After you have started the SST software, you can use the commands in the SST menu to collect sample and background data. Follow these steps:

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

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

Note Time-Resolved Step Scan experiments are available if you purchased the optional OMNIC SST with TRS Experiments software package. ▲

- 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 peak, or sample spacing parameters using one of the SST setup screens, it changes that parameter for all SST and standard OMNIC data collection techniques. ▲

- 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. 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 any spectrum.**

If you wish to ratio a group of 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 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 selected.

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

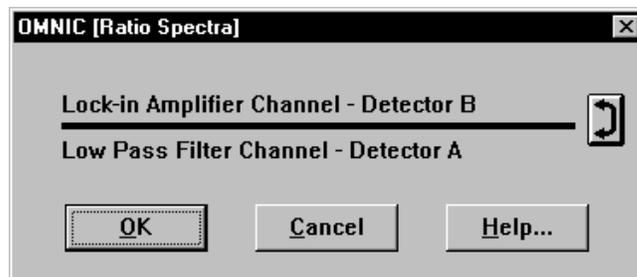
The special case of ratioing only two spectra

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. Here is an example:



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 allow you to reprocess (using the commands in the OMNIC Process menu) spectra collected using PM step-scan, PEM 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 about the central peak maximum. Each phase angle in the array is defined by the following equation:

$$\phi_i = \arctan(I_i / R_i)$$

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 data collected by the detector. During the conversion of an interferogram to a spectrum that can be analyzed, the apodization and zero filling operations that you selected using Experiment Setup, the Fourier transform operation, and the phase correction operation are performed.

The phase correction is calculated using the following formula:

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

where R_i and I_i are the real and imaginary points from the Fourier transform of the entire interferogram at frequency i , ϕ_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 PEM step scan, TRS step scan and PEM, 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 will be 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 selected Interferogram as your final format:

Use Open in the File menu to display the interferogram in a spectral window. The interferogram is selected automatically.

If you chose to save the interferograms with your spectrum:

Use Open in the File menu to display the spectrum in a spectral window.

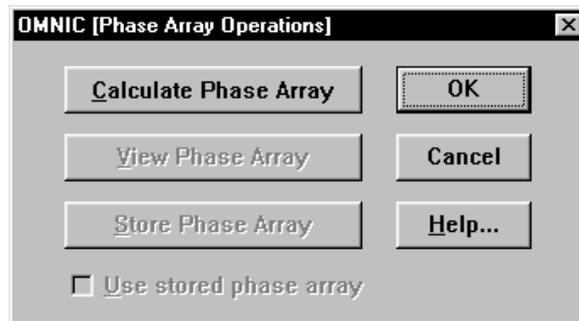
Choose Reprocess from the Process menu.

Select Interferogram from the Final Format drop-down list box.

Choose OK. The interferogram appears in a spectral window.

3. Choose Phase Array Operations from the SST menu.

The Phase Array Operations dialog box appears.



4. Choose Calculate Phase Array.

5. Configure OMNIC to use the stored phase array.

Turn on the Use Stored Phase Array check box and then choose OK.



OMNIC will use that stored phase array to process all subsequent interferograms until you turn the check box off or store another phase array.

Viewing a phase array

You must calculate the phase array before you can view it. Follow these steps:

- 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.

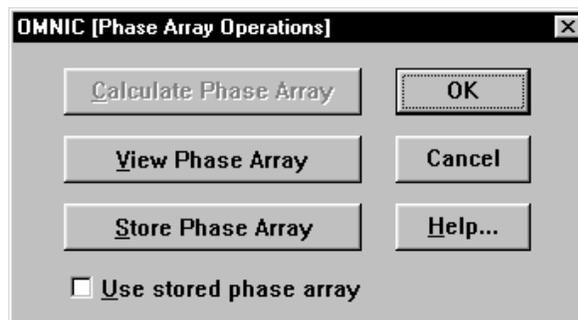
Storing a phase array

You must calculate and view the phase array before you can store it. Follow these steps:

- 1. Select the 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 is stored in memory, from which you can use it to process interferograms.

4. Configure OMNIC to use the stored phase array.

Turn on the Use Stored Phase Array check box and then choose OK.

Use stored phase array

OMNIC will use that stored phase array to process all subsequent interferograms until you turn the check box off or store another phase array.

Saving a phase array

You must calculate and view the phase array before you can save it. Follow these steps:

1. Select the phase array.

2. Save the phase array.

Use the Save As command in the File menu.

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.

The phase array will be saved as a standard OMNIC spectral data file. You can open it using any program that can read OMNIC files.



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. The Nexus system uses E.S.P. technology to identify each Smart Accessory as soon 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.



In Spectrometer Help Topics view “Installing a Smart accessory” in the “Installing optional hardware” book for instructions on installing Smart Accessories.

Nexus Smart ARK™ – This is a horizontal ATR 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 an aluminum, cast body for exceptional stability.

Nexus 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.

Nicolet Near-IR FiberPort™ – This accessory is optimized for near-IR sampling. The probe combines input and collection fibers in a unique sampling tip. In reflectance mode, solids and light-scattering liquids can be analyzed through direct contact. Transflectance mode is used for transparent liquids. This accessory is useful for the nondestructive study of polymers, pharmaceuticals, foods, fabrics and chemicals, as well as biological and environmental samples. The accessory uses an optimized lead sulfide detector.

Nicolet 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.

Nicolet Smart MIRacle™ – This 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.

Nicolet 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.

Nicolet 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.

Nicolet 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.

Nicolet Near-IR UpDRIFT – This is a top-loading diffuse reflection accessory designed for fast analysis of solids and powders. In many cases you can analyze samples directly from plastic or glass containers.

Nicolet 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.

Avatar™ Single-Bounce HATR – This is a single-reflection horizontal ATR accessory that has a shorter pathlength and higher throughput than traditional HATR accessory design. It is the best choice for routine analysis of strong infrared-absorbing samples. This is an economical choice for quality control or academic environments where routine analyses of neat solvents, aqueous solutions, powders and film samples are required.

Avatar Multi-Bounce HATR – This is a multi-reflection horizontal ATR accessory that has a shorter pathlength and higher throughput than traditional HATR accessory design. 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.

Avatar 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.



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

Other sampling accessories for different applications

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

Most accessories fit into the sample compartment, but some require separate housing and optics. Nicolet offers auxiliary experiment modules, microscopes, gas chromatography interfaces and thermogravimetric analysis interfaces with the Nexus 870.

Some accessories have their own optics. The optional mirror optics inside the spectrometer redirect the light beam from the internal light source through a port on the right side of the spectrometer. The beam then travels into the accessory’s optics.



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

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

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

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.

Continuum™, InspectIR™ and Advantage infrared microscopes – Nicolet offers microscopes that attach directly to either side of the spectrometer. Microscopes can also be installed between the spectrometer and other accessory modules. The microscopes provide fast, nondestructive microanalysis with minimal sample preparation and alignment. The beam path is switched from the spectrometer to the microscope module through the OMNIC software.

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 Nexus 870 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.

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.

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. The optional OMNIC SST with PEM Experiments software package is required for these experiments.

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.

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 – 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.

Transmission E.S.P. – 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 or an auxiliary experiment module.

TRS kits – Each TRS (time-resolved step-scan) 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 Nicolet's System Validation 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.

System accessories

Some system accessories are installed by Nicolet. Call Nicolet 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.

Uninterruptable power supply – An uninterruptable power supply reduces the chance of a system shutdown if power is lost elsewhere in the building.

Pure air generator – Nicolet offers a complete dry-air generation system. It includes an air compressor, a dryer, prefilters, a final filter/moisture indicator, and flow controls. If you have difficulty controlling moisture in your laboratory, the pure air generator provides additional protection for the hygroscopic elements of your spectrometer. This accessory is also useful if your laboratory environment 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, Nicolet 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.

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.

See the illustrations in the next sections for the locations of the connectors.

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.

Warning

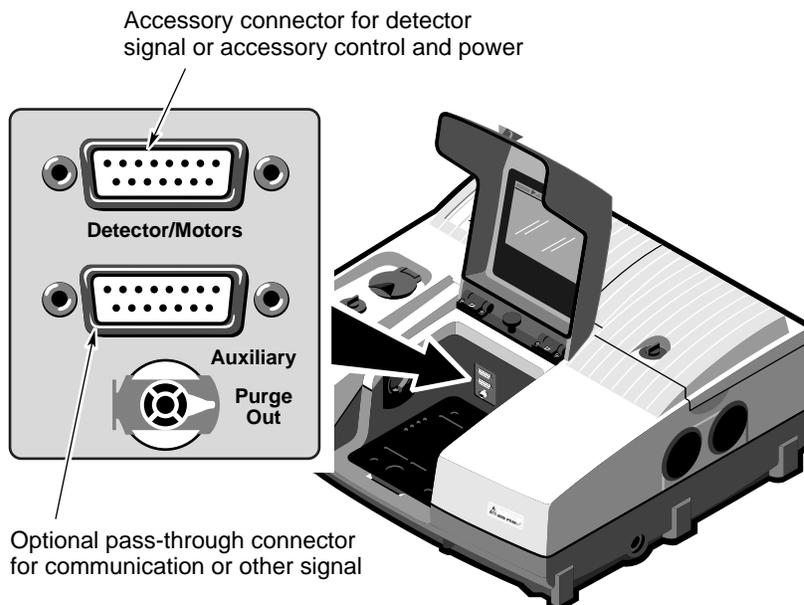
Improper or unsafe cabling can cause damage to your accessory and may create a safety hazard. Only qualified persons should cable a custom accessory using these connectors. Nicolet is not responsible for damage or injury resulting from improper or unsafe cabling. ▲

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.

See the next sections for details.

Connectors inside the sample compartment

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

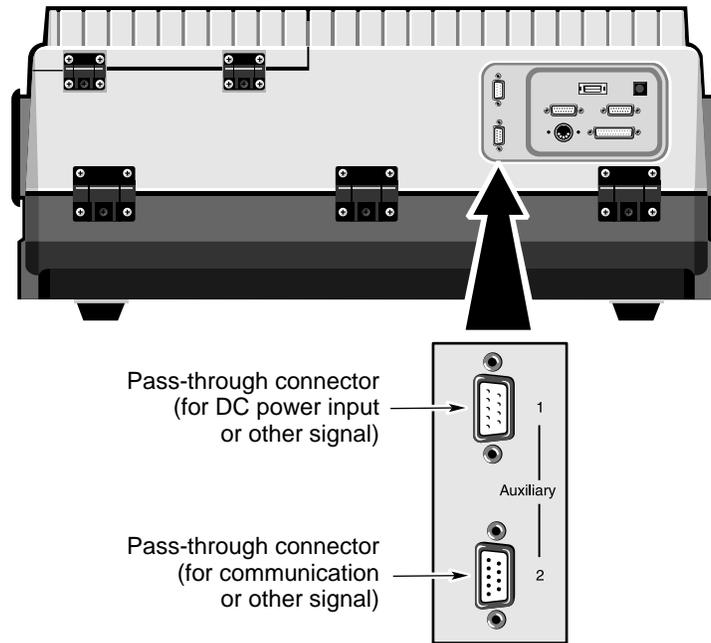


Detector/Motors – If you have a photoacoustic or other accessory that has a detector or motor located in the spectrometer sample compartment, connect the cable from the detector or motor to this standard connector. This is *not* a pass-through connector. See “Detector/Motors connector” for information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

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



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.

See the next section for information on which pins are available for use.

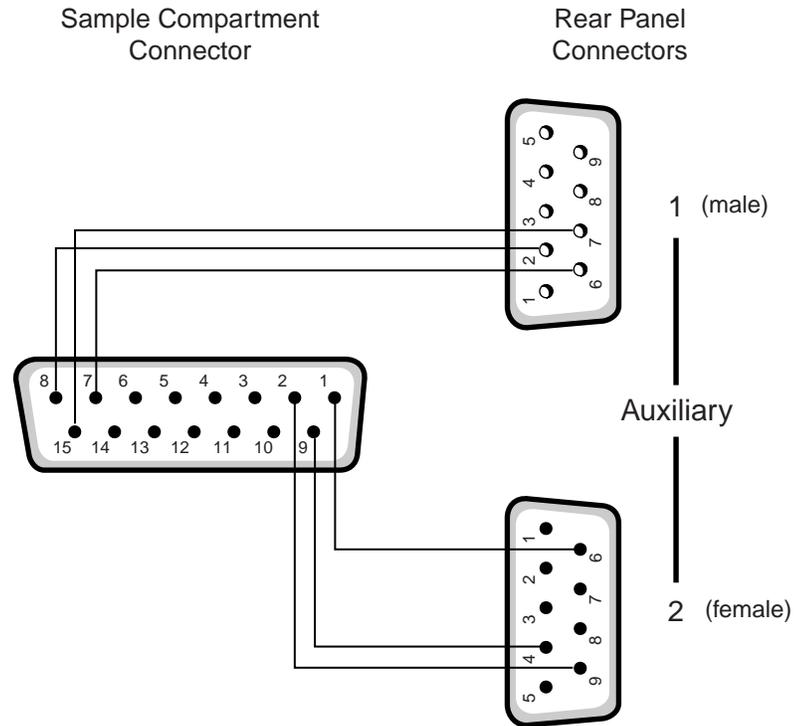
Using the pass-through
connectors for
custom accessories

By connecting custom cables that use the pins on the 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 rear panel to the sample compartment and vice versa. Make sure your use of the connectors complies with the voltage and current limitations given in the following Warning.

 **Warning**

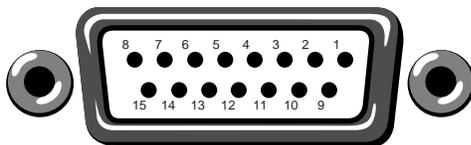
Improper or unsafe cabling can cause damage to your accessory and may create a safety hazard. Only qualified persons should cable a custom accessory using these connectors. Do not pass signals that exceed ± 15 VDC through these connectors. You must also limit the current to a maximum of 800 mA. Nicolet 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 rear panel. Since none of these connected pins are assigned by the Nexus 870, 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 to connect your own detectors, accessory motors and other custom hardware.



Detector/Motors

Make sure your use of the connector complies with the voltage and current limitations given in the following Warning.

⚠ 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 ± 15 VDC. Limit the current to a maximum of 800 mA. Nicolet is not responsible for damage or injury resulting from improper or unsafe cabling. ▲

The following table shows “pinout” information for the Detector/Motors connector. Use this information when designing a cable to connect your custom hardware to the connector. Refer to the preceding illustration for the locations of the numbered pins.

<i>Pin Number</i>	<i>Description</i>
1	Do not use this pin.
2	Used by the sample shuttle motor (negative).
3	Positive 5 volts.
4	Analog ground.
5	Used by the sample compartment detector for negative analog input.
6	Positive 12 volts analog.
7	Used by the sample compartment detector for digital communication.
8	Positive 5 volts.
9	Used for sample compartment digital communication.
10	Used by the sample shuttle motor (positive).
11	Positive 12 volts.
12	Analog ground.
13	Used by the sample compartment detector for positive analog input.
14	Negative 12 volts analog.
15	Used by the sample compartment detector for digital communication.



Quick 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 where to go for more information.

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.



Collecting a Spectrum (available through Learning OMNIC)...
“Preparing the Software”



In OMNIC Help Topics find “experiment” in the Index and go to “Selecting an experiment” or “Using Experiment Setup.”



SST Help Topics in the SST menu

How do I collect a spectrum?

Set the parameters as explained above and then choose Collect Sample from the Collect menu. Depending on the parameter settings, you may need to install or remove the sample before choosing Collect Sample.



Collecting a Spectrum (available through Learning OMNIC)...
“Collecting the Spectrum of a Sample”



In OMNIC Help Topics find “spectrum” in the Index and go to “Collecting a sample spectrum” or “Collecting a background spectrum.”



SST Help Topics in the SST menu

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.



Collecting a Spectrum (available through Learning OMNIC)...
“Typical IR Transmission Spectrum”



In OMNIC Help Topics find “units” in the Index and go to “Selecting the final format.”

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 raw data.



Collecting a Spectrum (available through Learning OMNIC)...
“Preparing the Software”



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

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.



Collecting a Spectrum (available through Learning OMNIC)...
“Collecting the Spectrum of a Sample”



In OMNIC Help Topics find “spectrum” in the Index and go to “Collecting a sample spectrum.”

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” in the Index and go to “Quality tab.”

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.



Collecting a Spectrum (available through Learning OMNIC)...
“Typical IR Transmission Spectrum”



In the OMNIC Help Topics Index...

Find “absorbance” and go to “Converting spectra to absorbance.”

Find “transmittance (%)” and go to “Converting spectra to % transmittance.”

Find “Kubelka-Munk units” and go to “Kubelka-Munk units.”

Find “photoacoustic units” and go to “Photoacoustic units” topic.

Find “reflectance (%)” and go to “% Reflectance units.”

Find “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 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.



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

- 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.



In OMNIC Help Topics find “blanking spectral region” in the Index and go to “Blanking a spectral region.”

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.)



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

- 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.



In OMNIC Help Topics find “Kramers-Kronig transformation” in the Index and go to “Kramers-Kronig (dispersion) transformation.”

- If you collected the spectrum using ATR (attenuated total reflection), use ATR correction (available through Other Corrections in the Process menu) to correct it for variation in the depth of penetration and then search it against a library of transmission spectra.



In OMNIC Help Topics find “ATR correction” in the Index and go to “ATR correction.”

- If the spectrum has water or carbon dioxide peaks, use Other Corrections to remove these peaks.



In OMNIC Help Topics find “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?

Use the Create Library button on the Library Names tab of Library Manager to create a user library.

Once a library is created, you can add spectra to it with the Add To Library button, 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.”

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

Locate and select the spectrum in Library Manager 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 can I find a compound in a commercial library?

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?

Use the Collect Spectrum button on the Library Names tab of Library Manager 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).



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

What does the search expert do?

It determines the spectral regions to search, searches those regions 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.



Collecting a Spectrum (available through Learning OMNIC)...
“Preparing the Software”



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

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 user library whose resolution is lower, the spectrum is deresolved. For this reason it may be better in some cases to save your sample spectra as files on the hard disk and consider the copies of them added to a user library to be 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 on 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 All (*.*) to see .NBK files listed. Select the file 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) to learn about OMNIC’s report features.



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 can also 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 have specified with Template or the template 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) 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 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?

By using the appropriate command, 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.



In the OMNIC Help Topics Index...

For information on Full Scale or Automatic Full Scale, find “spectra” and go to “Displaying spectra full scale” or “Displaying spectra full scale automatically.”

For information on Common Scale, find “spectra” and go to “Displaying spectra using the same Y-axis.”

For information on Match Scale, find “spectra” and go to “Matching the Y scale of a spectrum.”

For information on 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 click the top half of the Expand/Contract button at the left end of the view finder or drag the regions markers in the view finder to display a smaller spectral region.

In addition you can use the Roll/Zoom window available in the View menu (or click the Roll/Zoom Window button in the toolbar if displayed) to expand an area.



In OMNIC Help Topics find “spectrum” in the Index and go to “Selection tool,” “View finder” or “Rolling and zooming spectra.”

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.

You can also use the Roll/Zoom window available in the View menu to move a spectrum up or down.



In OMNIC Help Topics find “spectrum” in the Index and go to “Selection tool” or “Rolling and zooming spectra.”

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.”

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.



Collecting a Spectrum (available through Learning OMNIC)...
“Common Problems with IR Spectra”



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

Subtracting, adding, multiplying and dividing spectra

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.

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.

Note Subtract is available only when two spectra are selected. ▲

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. Here are some examples:

- 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).



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.



Collecting a Spectrum (available through Learning OMNIC)...
“Preparing the Software”



In the OMNIC Help Topics Index...

Find “options” and go to “Customizing OMNIC by setting options.”

Find “menu” and go to “Customizing a menu.”

Find “toolbar” and go to “Customizing a toolbar.”

Find “configuration” and go to “Saving a configuration.”

Find “configuration” and go to “Opening 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.

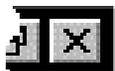


You can also use the annotation tool to label individual peaks.



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 feature in OMNIC, click the feature using the right mouse button. A brief description of the feature 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 feature (or the dialog box or window that contains the feature). 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 feature, 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).
- To see the Contents of the OMNIC Help system, choose OMNIC Help Topics from the Help menu.



Quick 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.



Spectrometer Help Topics...

“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.



Spectrometer Help Topics...

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

Does my detector need to be cooled with liquid nitrogen?

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.



Spectrometer Help Topics...
“Cooling a detector” in “Setting up experiments”

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.



Spectrometer Help Topics...

“Checking and changing desiccant” in “Maintaining your spectrometer”

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.

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). Nicolet 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.”



“Spectrometer Basics” chapter...

“Selecting the right 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.



See the “Troubleshooting” book in Spectrometer Help Topics 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.



“Diagnostics” chapter



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

How do I replace parts in the spectrometer?



Spectrometer Help Topics...
“Replacing parts”



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 Nicolet at one of the numbers below. Outside the U.S.A. call your local sales or service representative. Telephone numbers for all Nicolet Customer Support offices are provided with your system.

- Telephone (U.S.A.): 1-800-NICOLET (1-800-642-6538)
- Fax: 1-608-273-5045
- World Wide Web: <http://www.nicolet.com>
- E-mail: nicinfo@nicolet.com ▲



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

Aligning the spectrometer and accessories



This section describes how to use the OMNIC software to align the spectrometer and accessories.

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

Aligning the spectrometer

To ensure optimum system performance (high signal intensity, low noise and good sensitivity), you should occasionally align the spectrometer using the OMNIC software.

Note 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. ▲

Follow these steps:

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 can also 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 made available when you choose Spectrometer Help Topics from the Help menu. Call 1-800-NICOLET (1-800-642-6538) or 1-608-276-6373 to order the replacement assembly. If you are outside the U.S.A., contact your local Nicolet office. Telephone numbers for all Nicolet Customer Support offices are provided with your system.



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.
- Using remote diagnostics.

Checking the performance of spectrometer components

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 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. See “The OMNIC window” in the “Your First Experiment” chapter for more information. ▲

Follow these steps to run the spectrometer diagnostic tests:

1. Make sure the main sample compartment is empty.

Remove any samples and sampling accessories.

2. Choose Experiment Setup from the 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.

Running the spectrometer performance test

You can use the performance test to track long-term spectrometer performance. Run it after you have installed the system and then weekly. Keep a record of the actual 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.

Follow these steps:

1. Make sure the main sample compartment is empty.

Remove any samples and sampling accessories.

2. Exit OMNIC.

This ensures that the diagnostics software will run correctly.

3. Start the diagnostics software.

To do this, click the Start button in Windows, point to Programs, point to the OMNIC E.S.P. folder and then choose Bench Diagnostics.



See “Performing advanced diagnostic tests” for more information on running the diagnostics software.

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

Note If the noise readings are greater than normal or have changed significantly, call the Nicolet Customer Support Department for assistance. Outside the U.S.A., call your local service representative. Telephone numbers for all Nicolet Customer Support offices are provided with your system. ▲

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.

See “Running the remote diagnostics” for information about running performance tests for AM and PM step-scan experiments, PEM experiments, rapid scan, and the expanded spectral range available with your spectrometer

Performing 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 diagnostics software to:

- Run the spectrometer performance test.
- Test specific components of your spectrometer.
- Get information about replacement parts.
- Check the spectrometer configuration.
- Get troubleshooting tips.

Follow these steps to run the 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 E.S.P. 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.

Using remote diagnostics

The Nexus 870 is equipped with remote diagnostic capabilities. This includes a data modem and remote control software that allows control of your computer (and spectrometer) through the modem link. To take advantage of the remote diagnostic capabilities, you must have the modem connected to an analog telephone line.

Note We recommend that you dedicate a separate telephone line for data modem calls. If you require assistance, Nicolet Customer Support can discuss the problem with you through the voice line while running diagnostic tests on your system through the modem line. ▲

Remote diagnostic sessions

Follow these steps to start a remote diagnostic session:

1. Contact Nicolet and schedule a remote link.

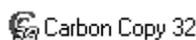
Remote links are provided only within the system warranty period or with an RSVP contract.

Note Steps 2, 3 and 4 must be completed before the scheduled remote link. The diagnostic session cannot begin until then. ▲

2. Exit the OMNIC software and close any open applications.

3. Start the remote control software.

Choose Start, point to Programs and then choose Carbon Copy 32 in the Carbon Copy folder.



4. Click the Wait For Call button.

You can also choose Wait For Call from the Connections menu.



5. Watch the screen while the remote session starts.

If you see any error messages, contact Nicolet Customer Support by telephone for assistance.

Note Once the remote session starts, do not use your computer unless the service engineer asks you to. When the service engineer is finished, the computer is returned to normal operating mode. ▲

Modem line specifications

The data modem requires an analog phone line (an outside line in most businesses). Many private branch exchange (PBX) phone systems use digital phone lines that will not work with your data modem. Ask your PBX administrator for a direct outside line or a sampled analog trunk line.

Use the following guidelines to determine whether or not you have an analog phone line.

Rotary phone – All rotary phones are analog phones. If you hear a dial tone when you plug a rotary phone into the phone wall jack, you have an analog phone line and your data modem will work.

Push-button phone – If you have a push-button phone, check the bottom of the phone to see whether it has a ringer equivalence number (REN) or a load number (LN). All analog phones have an REN or an LN. If you hear a dial tone when you plug a push-button phone that has an REN or an LN into the wall jack, you have an analog phone line and your data modem will work.

Wall jack specifications

In the U.S.A., install an RJ-11 jack; in Canada, install a CA11A jack. For other locations, contact your local Nicolet office for jack requirements.

Running the remote diagnostics

The Bench Diagnostics program includes performance tests for AM and PM step-scan experiments, PEM experiments, rapid scan, SMM and the expanded spectral range available with your spectrometer.

Note

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 E.S.P. folder.

5. Choose Performance Test.



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 Bench Diagnostics program includes performance tests for AM and PM step-scan experiments, PEM experiments, rapid scan, SMM and the expanded spectral range available with your spectrometer.

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 bench passed or failed the test.

Visible

Two visible spectral range tests are available. You must install and select visible-light hardware before you use this test.

1. Install a quartz beamsplitter, silicon detector and 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.

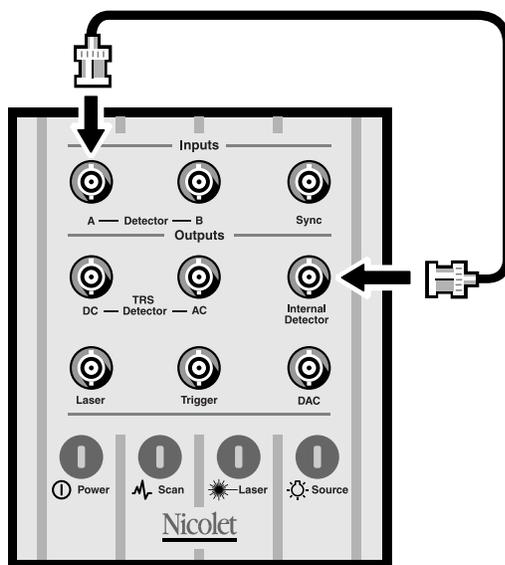
See “Installing optional hardware” in Spectrometer Help Topics for complete instructions for installing detectors, beamsplitters and filters.

2. Use OMNIC to select the visible light hardware.

AM step scan This test checks the amplitude modulation step-scan circuitry. You must install a cable and an energy screen before using this test.

1. Install the BNC-to-BNC cable.

Connect the cable between the Detector A and Internal Detector 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.

You do not need to set any AM setup parameters before running this test. Your parameters will be restored when the test is completed.

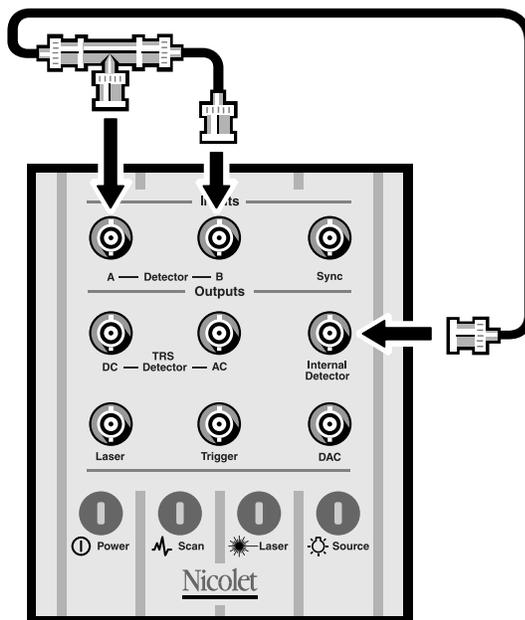
PEM This test checks the dual-channel circuitry. You must install cables before using this test.

1. Install the BNC “T” connector.

Connect it to the Detector A connector on top of the spectrometer as shown in the illustration in the next step.

2. Install the BNC-to-BNC cables.

Connect one cable between the BNC “T” connector and the Detector B connector on top of the spectrometer. Connect the other cable between the BNC “T” connector and the Internal Detector connector.



You do not need to set any PEM setup parameters before running this test. You may need to reset the parameters before running your next PEM experiment.

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

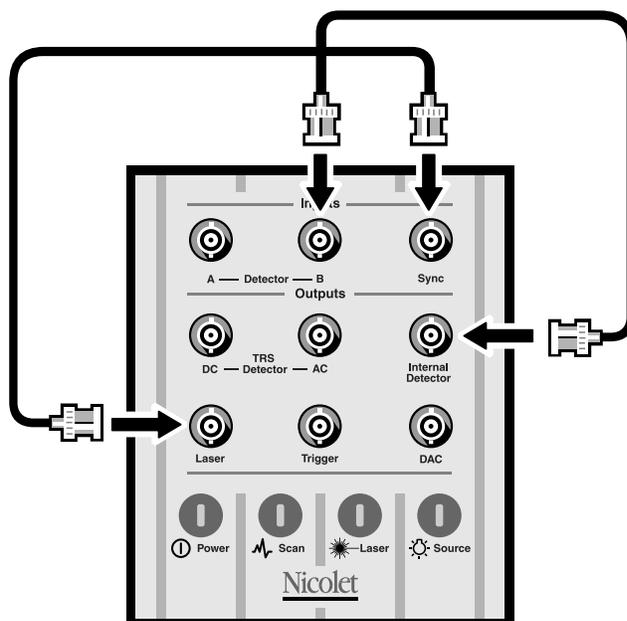
No cable connections are required, and you do not need to set any PM setup parameters before running this test. Your parameters will be restored when the test is completed.

SMM This test is a simulation of an SMM (synchronous multiple modulation) experiment. It verifies the basic operation of the spectrometer electronics.

This test requires cable connections.

Install the BNC-to-BNC cables.

Use one cable to connect the Internal Detector connector to the Detector B connector on top of the spectrometer. Use another cable to connect the Sync connector to the Laser connector on top of the spectrometer.



TRS This test checks the time-resolved step-scan circuitry in the optical bench and is available only if your system is equipped with the optional OMNIC SST with TRS Experiments software.

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.

1. Install the BNC “T” connector.

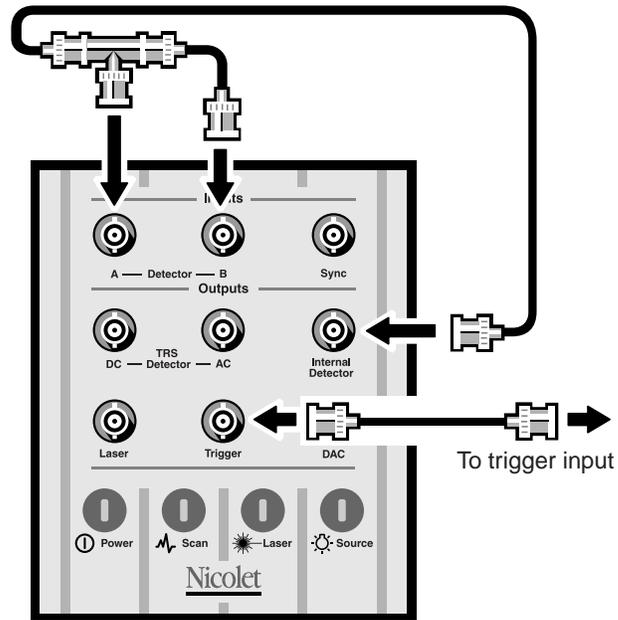
Connect it to the Detector A connector on top of the spectrometer as shown in the illustration in the next step.

2. Install the BNC-to-BNC cables.

Connect one cable between the BNC “T” connector and the Internal Detector connector on top of the spectrometer.

Connect a second cable between the BNC “T” connector and the channel 1 input on the data acquisition card (or the Detector B connector on top of the spectrometer, for internal TRS data collection).

Connect a third cable between the Trigger connector on top of the spectrometer to the trigger input (EXT) on the data acquisition card.



Note Choose Yes when prompted for information about the background source. ▲

▲ Caution 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. ▲



Troubleshooting Software Problems

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 your Nicolet service office.



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. No spectrum is selected. Quantitative analysis method is not appropriate for selected spectrum.	Select quantitative analysis method using Quant Setup in Analyze menu. Select single spectrum. Select appropriate method for selected spectrum.
You cannot add spectrum to user library.	Resolution of spectrum is lower (higher numerical value) than that of library.	Collect spectrum at same resolution as library (first set Resolution on Bench tab of Experiment Setup dialog box), and then add it to library.

Problem	Possible Cause	Solution
OMNIC needs to be restored after system crash, or message states that OMNIC cannot start or will no longer run.	There is not enough memory. There is another system problem.	Make sure OMNIC has enough memory. Quit other programs to free memory for OMNIC. Restart Windows. Run SCANDISK utility included with your Windows software. Restart OMNIC. If OMNIC does not start, reinstall it.
Experiment provided with OMNIC does not produce good results.	Parameter settings in experiment file have been changed so that experiment is no longer useful.	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 directory.
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 Problems

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 an message alerting you to the problem.



If the indicator is a yellow circle, a cooled detector in the Nexus 870 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. Power cable or power supply is defective.	Make sure power cord is plugged into spectrometer and working wall outlet. Check power LEDs on rear panel. All LEDs light when power supply is working properly. Call Nicolet to order replacement part.
Data are not displayed during collection.	Laser is not functioning. Data cable between spectrometer and computer is not properly connected.	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. Turn spectrometer power off and check data cable connections.
Source status indicator is off.	Source is burned out.	Call Nicolet to order replacement source. 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 Nicolet for service.

Problem	Possible Cause	Solution
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 Nicolet for service.
Baseline is not stable.	Purge rate is too high. Center laser detector is misaligned. Desiccant is expired. Spectrometer cover was recently opened.	Lower purge rate until baseline is stable. 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. If levels remain out of tolerance, call Nicolet for service. Replace desiccant. 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. Order replacement source if needed.

Problem	Possible Cause	Solution
System scans but gives very low signal intensity.	<p>Spectrometer is out of alignment.</p> <p>Detector and beamsplitter are not compatible.</p> <p>There is no interferogram.</p>	<p>Align spectrometer using Align button on Diagnostic tab in Experiment Setup dialog box.</p> <p>Make sure that selected detector and beamsplitter are compatible. Change detector or beamsplitter if necessary.</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. 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>
You encounter problems when selecting external detectors on AEM, GC interface or microscope.	<p>Custom detector is selected 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>Set Detector to None on Bench tab of Experiment Setup dialog box.</p> <p>Check and tighten cables.</p>
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, remove beamsplitter and check beamsplitter center window for fogging (check clear area located in center of substrate). Replace beamsplitter if necessary.

Problem	Possible Cause	Solution
Laser status indicator is off.	Beamsplitter compartment cover is not fully closed. Laser is burned out.	Close beamsplitter compartment cover. Call Nicolet to order replacement laser. View “Replacing the laser” in “Replacing parts” in Spectrometer Help Topics to find part number and ordering and installation instructions.
Scan status indicator does not flash (system is not scanning).	Spectrometer is out of alignment. After 1 hour without data collection activity, interferometer stops scanning and Scan light stays on. This mode is normal. Beamsplitter is not properly seated. Beamsplitter compartment cover is ajar. Electronic miscue has occurred. Component has failed.	Align spectrometer using Align button on Diagnostic tab in Experiment Setup dialog box. No action is required. Any data collection activity will cause interferometer to begin scanning. Check beamsplitter and reposition it if necessary. Close cover and tighten latch. Press Reset button on rear panel. Call Nicolet for service.

Problem	Possible Cause	Solution
Error message appears when you try to scan.	<p>Light source is not working.</p> <p>Detector is not cooled.</p> <p>Interferogram peak is not located at 1024 ± 16 data points on Bench tab in Experiment Setup dialog box.</p> <p>Beam path is blocked.</p> <p>Data cable between spectrometer and computer is not properly connected.</p> <p>Detector and beamsplitter are not compatible.</p>	<p>Check Source status indicator. If light is out, replace source.</p> <p>Check and cool detector.</p> <p>Align spectrometer. If interferogram is still not located correctly, call Nicolet for service.</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> <p>Turn off spectrometer power and check data cable connections.</p> <p>Change detector or beamsplitter.</p>



Troubleshooting Applications Problems



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 during the collection and other information about the collection.

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, call your Nicolet service office.



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. Infrared beam was reflected from (instead of penetrating) flat, shiny sample measured using specular reflection accessory.	Correct spectrum by using Other Corrections in Process menu. (Select Kramers-Kronig.) 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. Allow system three to five minutes to reestablish purge before collecting spectrum.
There are no peaks in spectrum.	There is no sample in infrared beam path. Sampling cup in diffuse reflection experiment is not in place or is tilted. Infrared microscope is in its viewing mode. Sample film in attenuated total reflection (ATR) experiment is being held against ATR crystal with uneven pressure or has poor contact with crystal.	Check sample compartment or accessory to make sure sample is properly positioned in beam path. Make sure cup is properly positioned in diffuse reflection accessory. Put microscope in infrared mode and collect spectrum again. Make sure sample is held evenly and has good contact with crystal.
Spectrum contains water peaks.	Spectrometer is not adequately purged. Desiccant is expired.	Make sure you are using correct purge gas and that purge flow rate is adequate. Allow system 3 to 5 minutes to reestablish purge before collecting spectrum. Check desiccant and replace it if needed.

Problem	Possible Cause	Solution
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.	<p>KBr pellet was made with coarsely ground KBr powder, or KBr pellet was improperly pressed.</p> <p>Background spectrum for cast film was collected with empty sample holder in infrared beam.</p> <p>Spectrometer is not properly aligned, causing sloped baseline.</p> <p>Spectrometer has not been on long enough to reach thermal equilibrium.</p> <p>Spectrometer is not properly purged.</p>	<p>Be sure to press pellet properly.</p> <p>Remove sample holder and collect background again.</p> <p>Use Align button on Diagnostic tab in Experiment Setup dialog box to align spectrometer.</p> <p>For best results allow spectrometer at least one hour to stabilize after turning it on.</p> <p>Check system to make sure correct purge gas is being used and that flow rate is correct.</p>

Problem	Possible Cause	Solution
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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