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MAGNA-IR®

FT-IR SPECTROMETERS

E.S.P.

System 560 and 760 User's Guide

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The Sync module on the Smart accessory baseplate is a factory-programmed, read-only device that does not allow a write operation from the spectrometer.

269-081600

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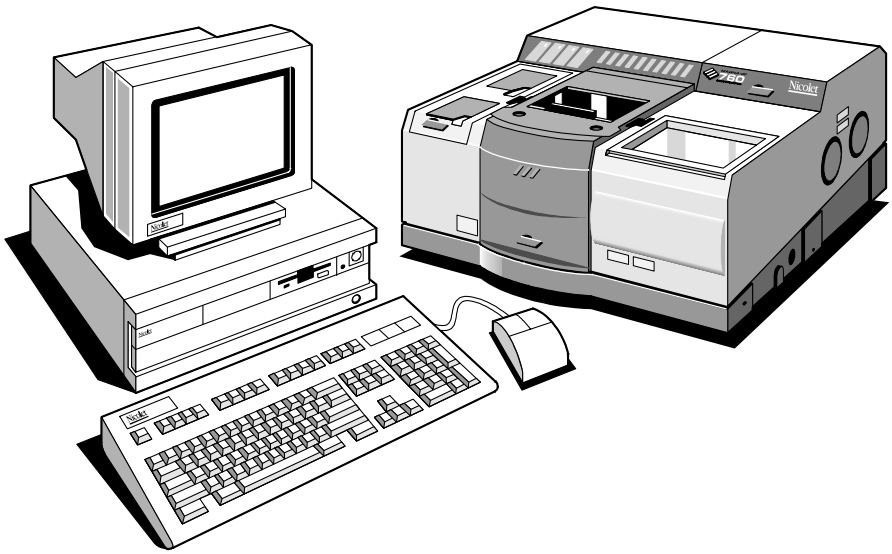
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Welcome

Congratulations on your purchase of a Magna-IR® E.S.P.™ System 560 or 760 spectrometer! The spectrometer lets you collect spectra in the mid-IR, near-IR, visible and far-IR spectral ranges. The E.S.P. system integrates the advanced hardware features of the Magna-IR spectrometer with the power and flexibility of Nicolet's OMNIC® software*.



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

---

* Some dedicated systems, such as the Liquid Analysis System, use other Nicolet software packages.



If you have not used the spectrometer before, use the "Getting Started" tutorial available in the Help menu of OMNIC or 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.

If you have questions, 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: 1-608-273-6045
- World Wide Web: http://www.nicolet.com
- E-mail: nicinfo@nicolet.com ▲

⚠ Warning The *Optical Bench 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 you use the system, read the entire guide. To prevent personal injury and damage to equipment, follow the safety precautions contained in the guide whenever you use the system. ▲

Conventions used in this manual

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



This symbol (shown enlarged here) tells you that you can find more information in the on-line tutorials or OMNIC Help system. You can access all of the on-line tutorials as well as the Help system by clicking the Help menu in OMNIC.

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. ▲

Where to find the information you need

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

Note The on-line tutorials are available only if you are using Windows 95 or Windows NT 4.0. ▲

The tutorials teach you how to do these things:

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

Note You must have the Spectrometer Tutorials CD in the computer to use the Spectrometer Tour or any parts replacement tutorials. ▲

You can also check parts lists or find other information without using the computer connected to the spectrometer. Insert the Spectrometer Tutorials CD into any Windows 95 computer and double-click the icon for the following programs to see information:

P560_ENU.HLP	Part numbers and replacement procedures for a 560 system
P760_ENU.HLP	Part numbers and replacement procedures for a 760 system
S560_ENU.EXE	Spectrometer tour for a 560 system
S760_ENU.EXE	Spectrometer tour for a 760 system

To use a tutorial, point to Learning OMNIC in the Help menu and then choose the desired tutorial from the list that appears. Tutorials also appear in these Help menus: Replacing Parts, Installing Hardware and Troubleshooting. You can also start tutorials from within other parts of the on-line documentation provided with OMNIC.

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

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:

- If you have Windows 95 or Windows NT 4.0, you can see information about a particular feature in OMNIC (such as a menu command, a parameter in a dialog box, etc.) 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. 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 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.

Use the following sections to help you locate the information you need.

The basics

How do I turn on the system?



View the “Powering Up” unit of the “Spectrometer Tour” tutorial.

See “Turning on the system components” in the “Before You Collect Spectra” chapter of this manual.

How do I start the software?

See “Starting OMNIC” in the “Before You Collect Spectra” chapter of this manual.

How do I prepare the software for data collection?



View the “Preparing the Software” lesson of the “Collecting a Spectrum” tutorial.

How can I learn how to use the software?



View the tutorials listed when you point to Learning OMNIC in the OMNIC Help menu.

What hardware and software do I need?

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

- Intel® Pentium® processor with 100 MHz or greater clock speed.
- At least 16 megabytes of random access memory (RAM).
- The capability of displaying at least 256 colors.
- 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.
- A 16-bit Sound Blaster-compatible sound card.
- Two serial ports.
- An ECP bidirectional parallel port.
- Three ISA/PCI slots.
- One of the following versions of Windows™ software:
  - Windows 95 (recommended, provides all the features)
  - Windows NT 4.0 or greater (recommended NT version, can be used on a workstation system or with a Magna-IR or Protégé spectrometer)
  - Windows NT 3.51 or greater (minimum NT version, can be used only on a workstation system)
  - Windows 3.1 or greater (minimum version, does not provide all the features)

Using the spectrometer and changing parts

What's inside the spectrometer?

How does the spectrometer work?



For an overview of the theory behind FT-IR, see the "Beginner's Guide to FT-IR" tutorial.

How do I purge the system?



View the "Purging the optical bench" lesson in the "Preparing Your Optical Bench" unit of the "Collecting a Spectrum" tutorial.

See also instructions for using the Purge Curtain in the "Sample Compartment" lesson of the "From the Front" unit of the "Spectrometer Tour."

How do I change beamsplitters?



Choose Replacing Parts from the OMNIC Help menu and view the "Changing beamsplitters" tutorial in the "Replacing parts" book.

See "Selecting the right beamsplitter and detector" in the "Using beamsplitters and detectors" section of the "Optical Bench Basics" chapter of this manual for tables showing the compatibility of sources, beamsplitters and detectors.

How do I change detectors?



Choose Replacing Parts from the OMNIC Help menu and view the "Changing detectors" tutorial in the "Replacing parts" book.

See “Selecting the right beamsplitter and detector” in the “Using beamsplitters and detectors” section of the “Optical Bench Basics” chapter of this manual for tables showing the compatibility of sources, beamsplitters and detectors.

How do I install a source?



Choose Replacing Parts from the OMNIC Help menu and view the “Changing your source” tutorial in the “Replacing parts” book.

See “Selecting the right beamsplitter and detector” in the “Using beamsplitters and detectors” section of the “Optical Bench Basics” chapter of this manual for tables showing the compatibility of sources, beamsplitters and detectors.

Collecting spectra

Which beamsplitter and detector should I use?



Choose Replacing Parts from the OMNIC Help menu. Then view the “Selecting a beamsplitter, detector, and source” tutorial in the “Replacing parts” book for tables showing the compatibility of sources, beamsplitters and detectors.

See “Selecting the right beamsplitter and detector” in the “Using beamsplitters and detectors” section of the “Optical Bench Basics” chapter of this manual for these tables.

How do I install a sample?



View the “Installing samples” unit of the “Spectrometer Tour” tutorial.

How do I collect a spectrum?



View the "Collecting a Spectrum" tutorial, listed when you point to Learning OMNIC in the OMNIC Help menu.

See the "Your First Experiment" chapter of this manual for a lesson on collecting spectra.

Accessories

What accessories are available?



View the "Accessories" unit of the "Spectrometer Tour" tutorial for a general description of the available accessories, or see the "Accessories You Can Buy and How to Install Them" chapter of this manual.

How do I install an accessory?



Check the "Installing optional hardware" and "Replacing parts" help books listed when you choose Installing Hardware in the OMNIC Help menu. These help books provide step-by-step instructions and, in many cases, on-line videos to help you install accessories. If the accessory you purchased is not covered on-line, use the instructions that come with the accessory.

Maintenance and service

How should I maintain my spectrometer?



View the "Service and maintenance" unit of the "Spectrometer Tour" tutorial for information on maintaining the spectrometer. You can also choose Replacing Parts from the OMNIC Help menu and view the tutorials in the "Maintaining your optical bench" book.

See the "Service and Maintenance" chapter of this manual for information on maintaining the spectrometer.

What should I do if there is a problem with the system?

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: 1-608-273-6045
- World Wide Web: http://www.nicolet.com
- E-mail: nicinfo@nicolet.com ▲

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 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 indicator.
- Make sure the system components are on.
- Cool the detector (if required).
- Open an experiment.

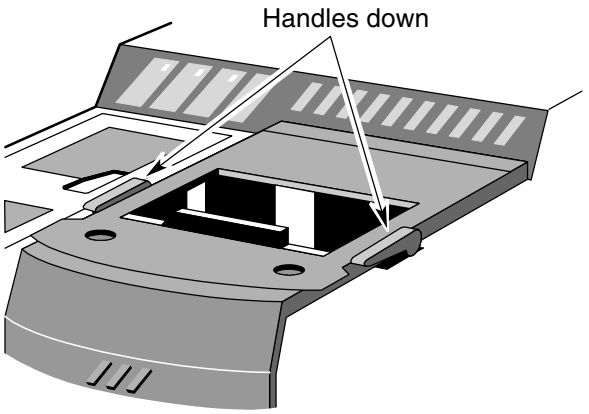
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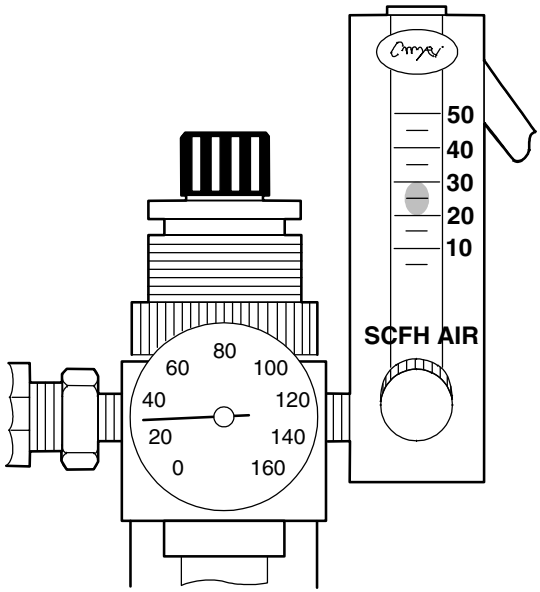
Checking the purge

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

If your spectrometer is purged, make sure both purge shutters are open (handles in the down position) whenever the sample compartment door is closed. This allows the purge gas to flow between the sample compartment and the rest of the spectrometer so that the entire spectrometer is purged.



Also make sure the pressure regulator is set between 20 and 40 pounds per square inch (psi) and the flowmeter is set to 25 standard cubic feet per hour (scfh).



⚠ 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. We recommend using dry air or nitrogen. ▲

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.

Choose Installing Hardware from the OMNIC Help menu and view the tutorials in the "Maintaining your optical bench" book for information on how to install the purge equipment, set the controls for the first time, and inspect and clean the purge filter. View the "Sample compartment" topic in the "Spectrometer Tour" for information on using the Purge Curtain.

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.

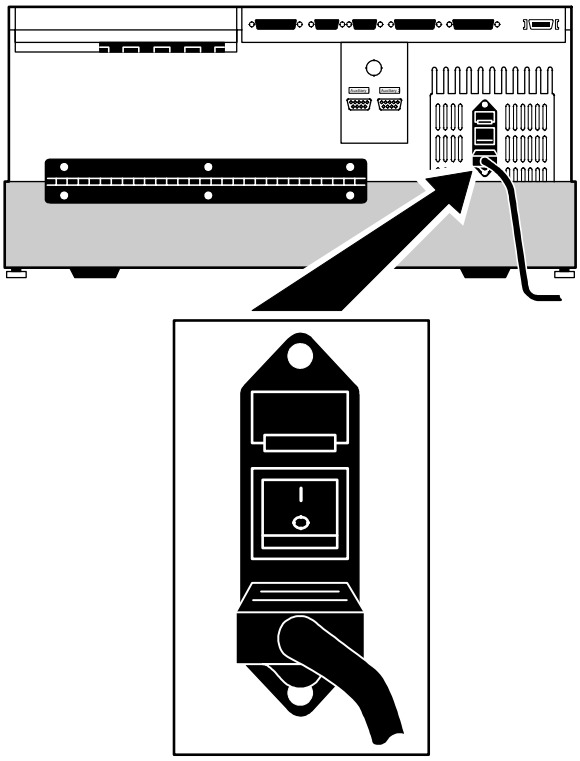
Follow these steps to turn on the system components:

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

   This includes accessories such as the Raman Accessory for Magna-IR, a gas chromatograph and GC interface, or an infrared microscope.

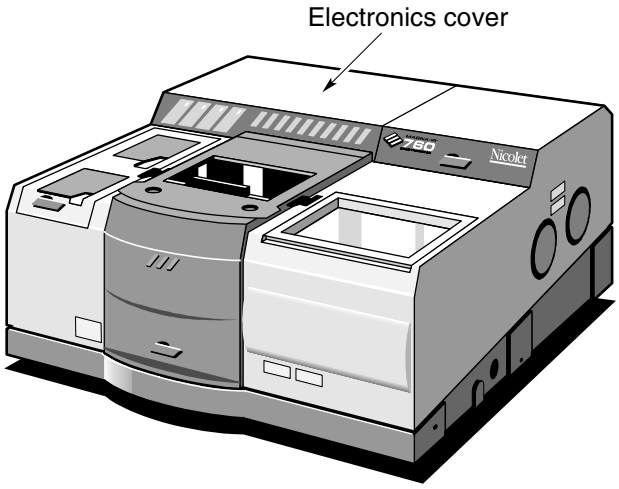
2. Turn on the spectrometer.

Press the power switch on the rear panel to |.



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

▲ **Caution** The electronics compartment is located under the cover in the top-left-rear corner of the spectrometer.



To avoid overheating the electronic components, do not place anything on top of the electronics cover. ▲

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 optical bench power" in the "Optical Bench Basics" chapter if you want more information on turning on the spectrometer.

3. Turn on the computer and printer.

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

Cooling the detector



Some detectors, such as an MCT or InSb detector, require cooling with liquid nitrogen. Choose Installing Hardware from the OMNIC Help menu and view the "Cooling a detector" tutorial in the "Installing hardware" book for information on how to cool an MCT detector.

⚠ 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, allow the detector to cool at least 20 minutes before collecting spectra.

Installing OMNIC

If you need to install OMNIC on your hard drive, follow these directions. The procedure for installing OMNIC depends on the version of Windows™ you are using.

If you have Windows 95 or Windows NT 4.0, follow these instructions:

Start your Windows software and insert the OMNIC CD into the drive.

The installation automatically starts.

If the Autorun setting is off, or if you are installing the software from floppy disks, use the Add/Remove Programs dialog box in Windows 95 to install OMNIC. Click the Start button and choose Control Panels from Settings. Double-click the Add/Remove Programs icon, and then choose the Install/Uninstall tab in the window. Click the Install button and follow the directions to install the OMNIC software.

If you have Windows 3.1 (or 3.11) or Windows NT 3.5, follow these steps:

1. **Start your Windows software and insert the OMNIC CD into the drive.**

2. **Choose Run from the Program Manager File menu.**

3. **Type *X:setup* (where X is the drive letter for your CD-ROM drive). Then press Enter.**

Starting OMNIC

The procedure for starting OMNIC depends on the version of Windows you are using.

If you have Windows 95 or Windows NT 4.0, follow these steps:

1. **Start your Windows software.**

2. **Double-click the OMNIC E.S.P. shortcut.**

   The OMNIC shortcut is on the Windows desktop.



   Depending on how the program has been configured, dialog boxes may appear asking for a user name and password. Type in 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.

If you have Windows 3.1 (or 3.11) or Windows NT 3.5, follow these steps:

1. **Start your Windows software and display the Program Manager window.**

2. **Open the group window that contains the OMNIC icon.**

   The OMNIC icon is normally located in the OMNIC group window. The icon looks like this:



   If the OMNIC group window is not open, you can open it by double-clicking its icon.

3. **Double-click the OMNIC icon to start OMNIC.**

   Depending on how the program has been configured, dialog boxes may appear asking for a user name and password. Type in 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 want to check or change the parameters after selecting an experiment, use Experiment Setup in the Collect menu.



To learn more about experiments, see the "Preparing the Optical Bench" lesson in the "Collecting a Spectrum" tutorial. If you need to install or change a source, beamsplitter or detector for your experiment, follow the instructions in the "Replacing parts" tutorial available in the OMNIC Help menu.

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. ▲



You are now ready to collect spectra. If you have not used the system before, you can learn how to perform an experiment by viewing the "Collecting a Spectrum" tutorial available in the Help menu of OMNIC or 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:

- Find the on-line tutorials, wizards and Help system.
- Open a configuration.
- Select an experiment and check the parameters.
- Install a sample and collect a sample spectrum.
- Label peaks in a spectrum.
- Search a spectrum against a library.
- Create and print a report.
- Add a spectrum to a user library.



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

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

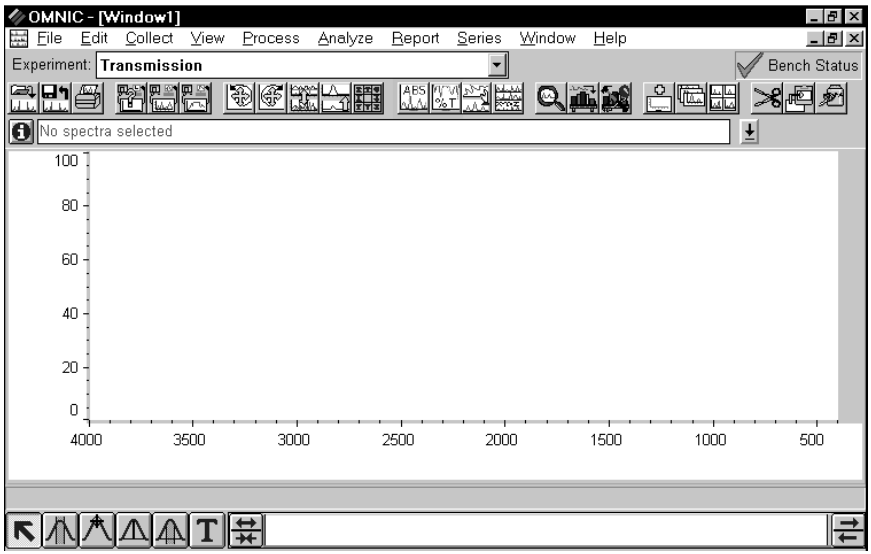
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- Fax: 1-608-273-6045
- World Wide Web: http://www.nicolet.com
- E-mail: nicinfo@nicolet.com ▲

Note If you have a dedicated system (such as an ECO/RS or a Liquid Analysis System) 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.



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.

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.

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.





To the right of the Experiment drop-down list box is the Bench Status indicator. The indicator is a green check mark when the spectrometer is operating properly. If there is a problem with the spectrometer, the indicator turns to a yellow circle or red X. A yellow circle indicates that the spectrometer has failed a performance test, but the failure is usually not serious enough to prevent you from collecting usable spectra. A red X indicates that the spectrometer has failed a performance test that requires corrective action. Diagnostic information appears allowing you to troubleshoot the problem.

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

Below the Experiment drop-down list box is the toolbar. Each button in the toolbar represents the action taken by a corresponding command or feature. To see the name of the command or feature for a button, point to the button and press the right mouse button. To initiate the command or feature, click the button with the left mouse button.

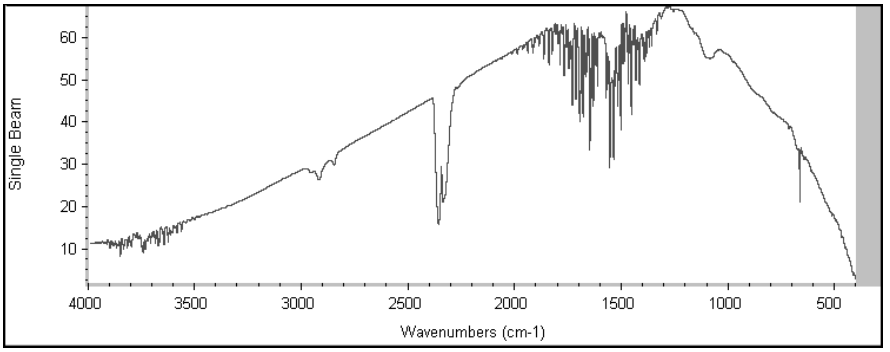


In the OMNIC Help system Index, find “toolbar” and go to the “Displaying and using a toolbar” topic for information on using and customizing the toolbar buttons.

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:



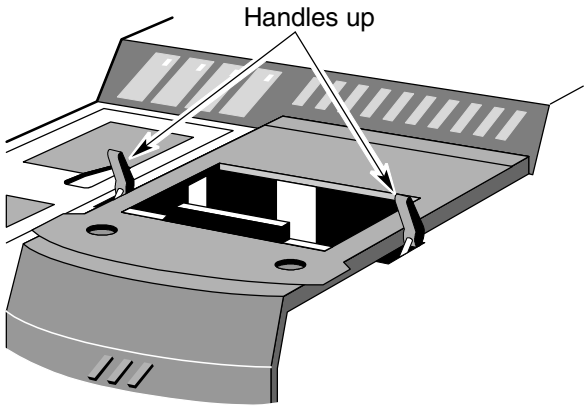
For most applications you don't need to collect a new background spectrum for each sample spectrum if you haven't changed the software parameters. To obtain good results, however, collect a new background regularly, perhaps once every four hours. (You can obtain the best results by collecting a new background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

1. **If your spectrometer is purged, close the purge shutters (handles in the up position).**

   This helps keep water vapor and carbon dioxide out of the spectrometer.

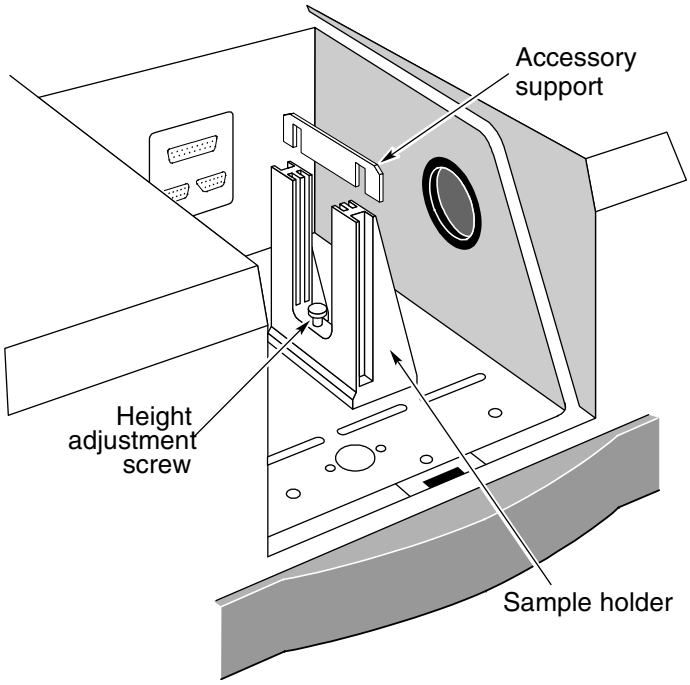




View the “Purging the optical bench” lesson in the “Preparing Your Optical Bench” unit of the “Collecting a Spectrum” tutorial if you want to read more about purging the spectrometer and using the purge shutters.

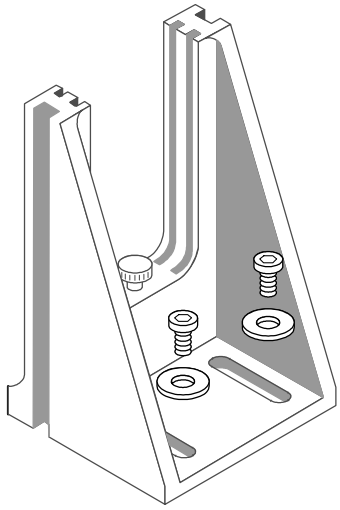
2. Install the sample holder.

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, choose Replacing Parts from the OMNIC Help menu. Then choose the "Removing the snap-in baseplate" topic from the "Replacing parts" book.

If your sample holder is not installed on a baseplate, use a flat bladed 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 preceding illustration). Replace the support when you are finished using the slot. *Do not discard the support; it is needed for installing slide-mounted accessories.*

3. **Close the sample compartment cover and its sliding door.**

4. **If your spectrometer is purged, open the purge shutters (handles in the down position).**

   Allow 1 minute for purge to be reestablished before collecting the polystyrene spectrum in the following procedure.

Collecting the sample spectrum

In the data collection procedure that follows, you will collect a background before collecting a polystyrene sample spectrum. By selecting one of the experiments provided with OMNIC, you will quickly select this background handling option as well as set other software parameters before you collect the spectra.

You will also open a configuration that sets a number of software options for this procedure.



You can also learn how to collect spectra by using the "Collecting a Spectrum" tutorial available through the Learning OMNIC item in the Help menu.

Follow these steps to collect the sample spectrum:

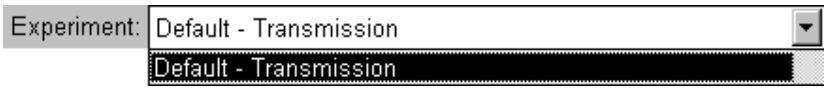
1. **Choose Open Configuration from the File menu.**

   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. **Click the arrow button at the right end of the Experiment drop-down list box.**



The Default - Transmission experiment appears in the list.

A number of other experiments are included for performing a wide variety of data collections. You can install experiments by choosing Open from the Experiment Setup dialog box. You can also set up and save your own experiments.

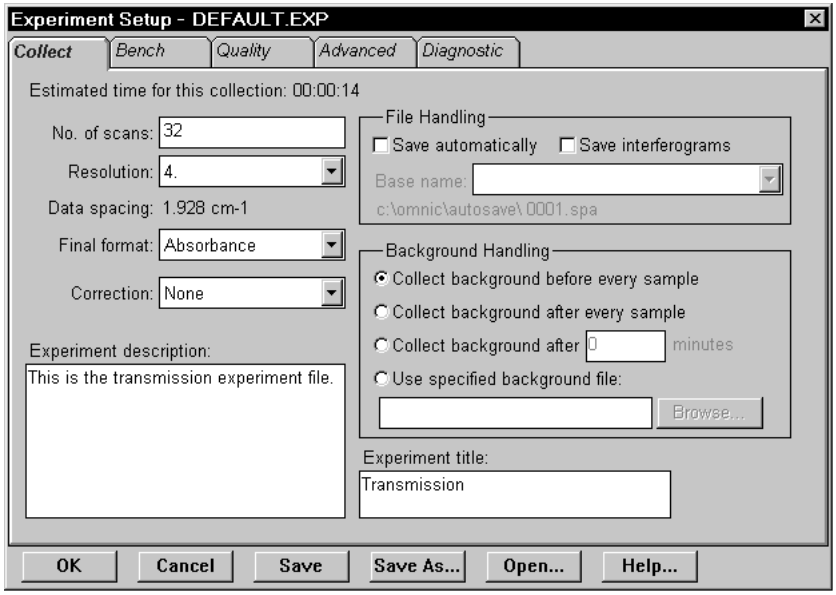
4. **Select the Default - Transmission experiment by clicking it.**

The parameters in the Experiment Setup dialog box are now set correctly for collecting a polystyrene sample spectrum.

5. **You can check the settings of the parameters by choosing Experiment Setup from the Collect menu.**

The Experiment Setup dialog box appears.

6. **Click the Collect tab to display the data collection parameters.**





The data collection parameters, along with the other experiment parameters, determine how OMNIC collects background and sample spectra. See the OMNIC Help system for complete information on the parameters.

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.

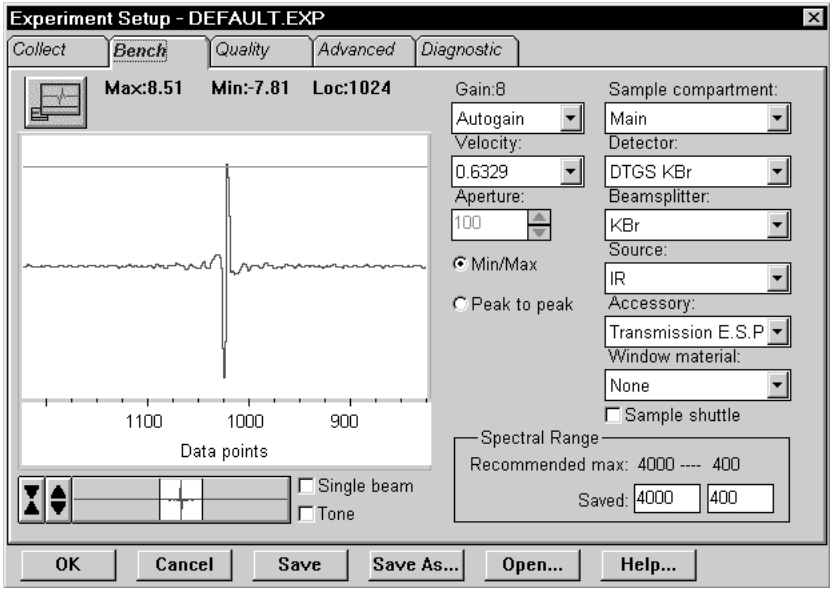
If Save Interferograms is on, the interferograms for your spectra are saved when you save the spectra. Interferograms are the raw spectral data. Saving them allows you to reprocess a spectrum later in case you want to restore it after performing corrections or other operations on the data.



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

7. 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.



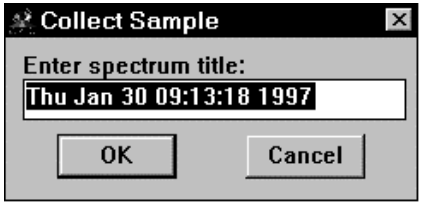
8. **Choose OK to close the Experiment Setup dialog box.**

   Now that you have selected the Default - Transmission experiment, you can collect a spectrum of the polystyrene sample.

9. **Choose Collect Sample from the Collect menu.**

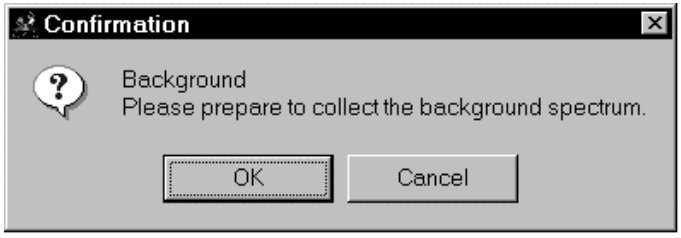


   You can also click the Collect Sample button in the toolbar to begin collecting the sample. The Collect Sample window appears and then a dialog box showing the default title for the sample spectrum:



10. **Type a title in the text box or choose OK to accept the default title for the spectrum.**

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

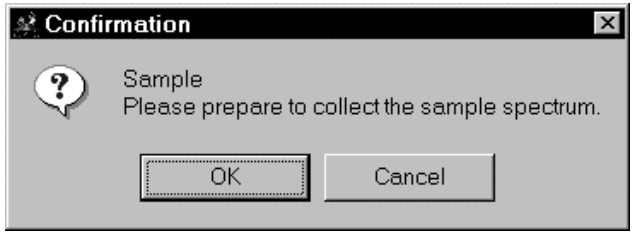


This means that you need to remove any sample from the sample holder so that the beam path is clear. When you then collect a background spectrum, the result is a measurement of the response of the spectrometer alone; that is, without absorptions due to a sample.

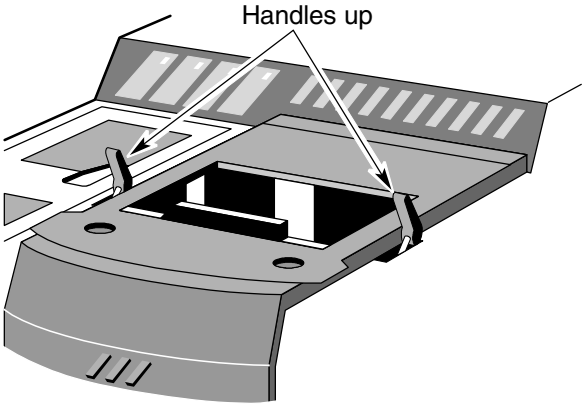
11. Look through the sliding door to make sure there is no sample in the sample holder and then choose OK to start data collection.

If there is a sample in the sample holder, close the purge shutters (handles in the up position), open the sliding door, remove the sample, close the sliding door, open the purge shutters (handles in the down position) and then wait 1 minute before choosing OK. The illustration in the next step shows the location of the purge handles.

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:



12. **If your spectrometer is purged, close the purge shutters (handles in the up position) before opening the sliding door in the next step.**



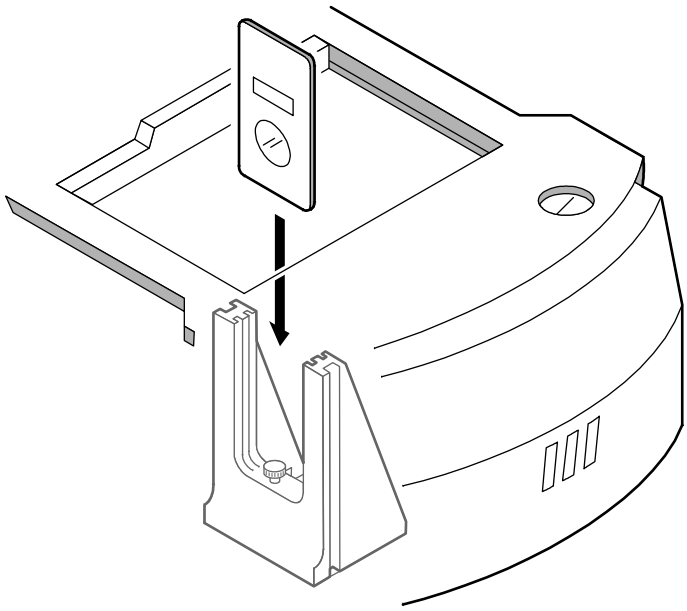


This helps keep water vapor and carbon dioxide out of the spectrometer. View the “Purging the optical bench” lesson in the “Preparing Your Optical Bench” unit of the “Collecting a Spectrum” tutorial if you want to read more about purging the spectrometer and using the purge shutters.

13. Install the polystyrene sample.

First open the sliding door.

Next insert the sample into the sample holder.



Then close the sliding door.



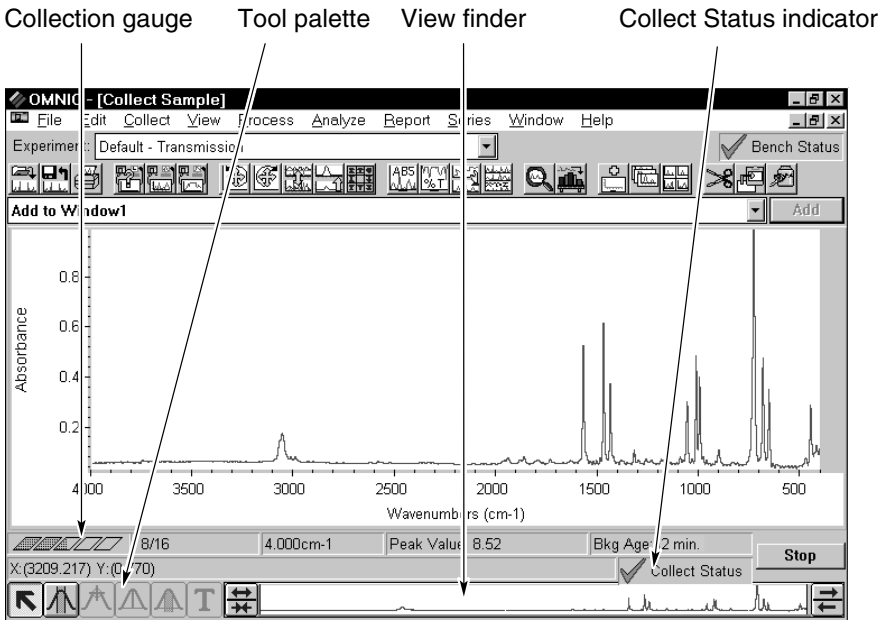
View the "Installing Samples" unit of the "Spectrometer Tour" tutorial for more information on installing samples.

14. If you closed the purge shutters earlier, open them (handles in the down position).

Allow 1 minute for the purge to reach equilibrium before going to the next step. If you had left the purge shutters open when you inserted the sample, you would need to wait 3 to 5 minutes.

15. Choose OK to start sample data collection.

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



Sample spectrum

16. Monitor the status of the data collection.

The progress of the collection is indicated visually by the collection 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.

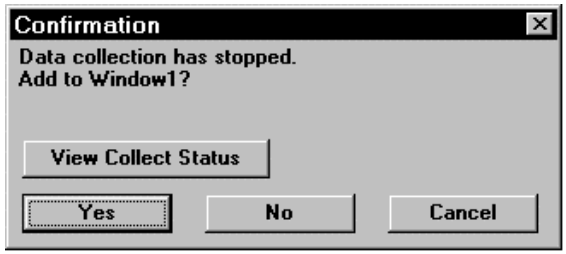
The Collect Status indicator above the view finder shows the status of the collection during and after collection. The indicator is a green check mark, showing that the spectrum has passed all of the selected spectral quality checks made so far. After the collection is finished and the indicator is a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

If you ever have a problem with data collection, 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:

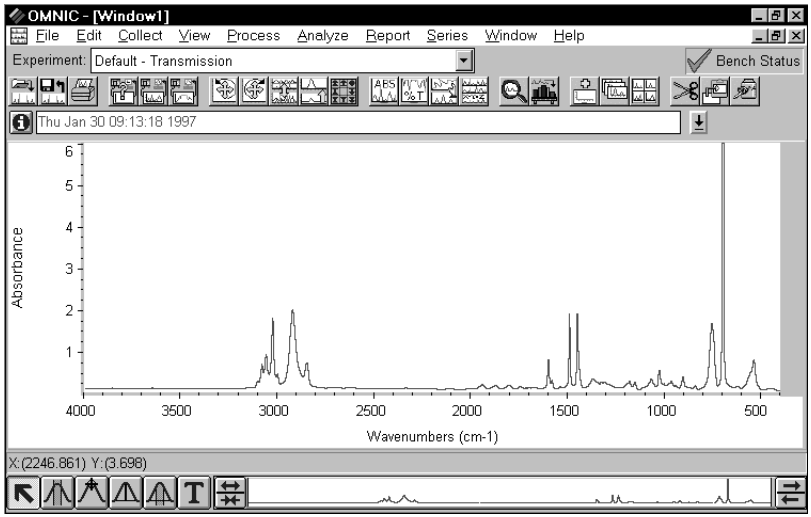


Clicking the View Collect Status button displays the Results window, showing a summary of any problems encountered during data collection and other information about the collection.

17. 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. This is a standard Windows dialog box.

3. **Type the name POLY.SPA following the directory path in the File Name box so that the text reads C:\OMNIC\SPECTRA\POLY.SPA.**

   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 absorbance.

Converting the spectrum's units

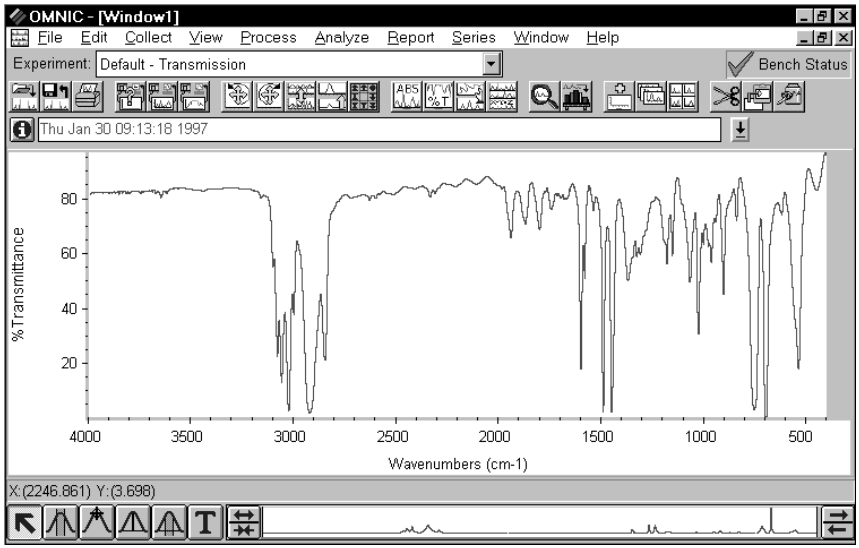
The polystyrene spectrum you collected is in absorbance units. Since many of OMNIC's data manipulation commands work best on spectra in absorbance units, it is useful to convert a spectrum to absorbance by using the Absorbance command. For this example you will convert the spectrum to % transmittance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

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



2. **Choose 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 the OMNIC Help system Index, find "converting spectrum" and go to the topic discussing the units to convert to.



3. Choose the Absorbance button in the toolbar.

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

Labeling a peak with the annotation tool

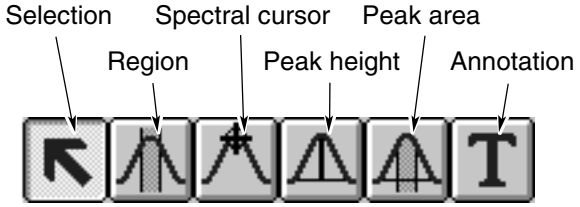
The palette contains six tools that let you select a spectrum or spectral region, change how spectra are displayed in a spectral window, find the height or area of a peak, or label a peak. The names and appearance of the palette tools indicate their functions.

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



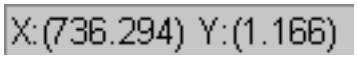
1. Select the annotation tool by clicking it on the palette.

The annotation tool in the palette 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:



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

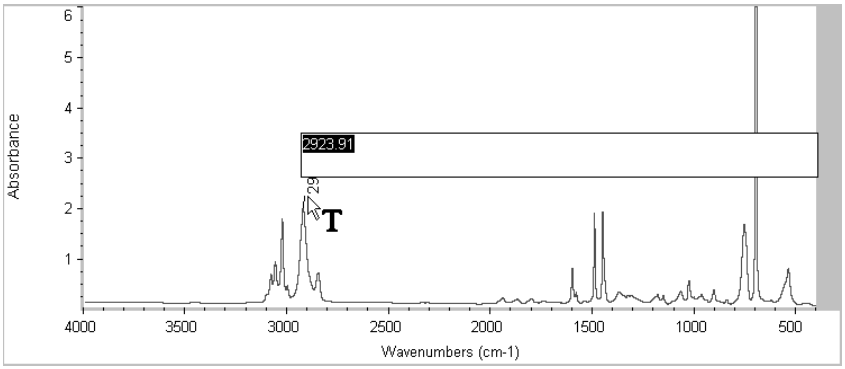


You can label a peak by clicking above it with the annotation tool. This displays the label text above the peak with a line connecting the label to the peak. The text is selected so that you can immediately edit it. When you press Enter, the label appears in its final form.

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.**

   To modify the label, edit the selected text before pressing Enter. To modify an existing label, select the Annotation tool and click the label you want to change. Type a new label.

   To delete a label, select the Annotation tool and click the label. Then press the Delete key.



In the OMNIC Help system Index, find "tool, annotation" and go to the "Annotation tool" topic for more information on the annotation tool.

In the next section, you will search the spectrum against a spectral library to identify it.

Searching a spectral library

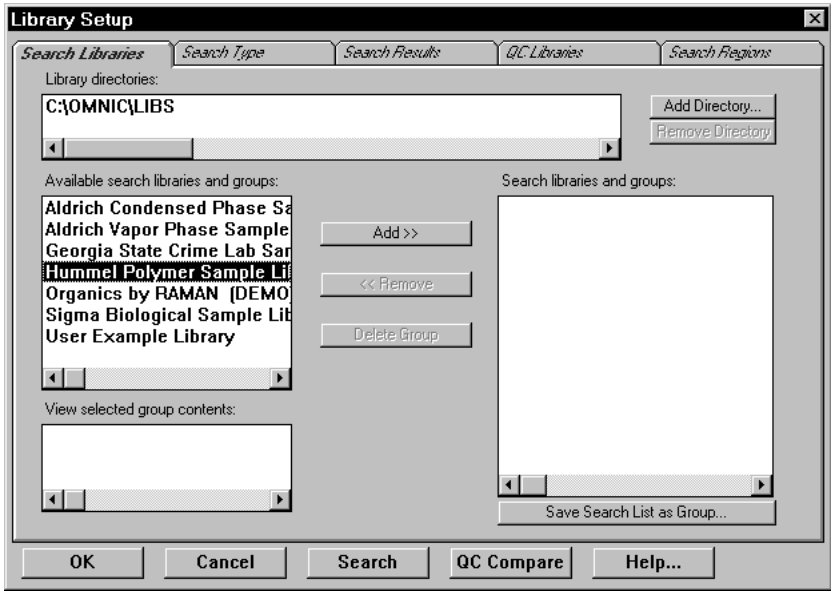
You already know that your sample is polystyrene, but if you were unsure of its composition, you could identify it by searching the sample spectrum against a spectral library that contains a reference spectrum of the same material.

Follow these steps to search the sample spectrum against a spectral library:

1. **Select the polystyrene spectrum.**

2. **Choose Library Setup from the Analyze menu.**

   The Library Setup dialog box appears with the Search Libraries tab displayed.



3. **Choose the directory that contains the libraries and library groups you want to search.**

   To add a directory to the search list, choose Add Directory. In the dialog box that appears, locate and select the C:\OMNIC\LIBS directory, and then choose OK. The available libraries are added to the Available Search Libraries and Groups box.

4. **Add one or more libraries to the Search Libraries And Groups box.**

   The libraries listed in the Search Libraries And Groups box are the libraries that your spectrum will be compared to. Click a library you want to add, and then click the Add button to add it to the Search Libraries And Groups box.

5. **Click the Search Results tab, and then select Use Search Expert.**

   Using the search expert saves you time because it always searches the region from 2600 to 450 wavenumbers. You can also choose to make more specific searches by selecting Configure Search Results and specifying the search parameters.

6. **Choose Search in the Library Setup dialog box.**

   You can also close the Library Setup dialog box and begin a library search at any time by choosing Search from the Analyze menu.

When you begin a library search, the Search window appears. At the bottom of the window a gauge shows the progress of the search. As library matches are found, the closest matches are added to the search results list in order of match value, with the best match listed first. Depending on which libraries you selected to search, you may or may not get a good match for the polystyrene spectrum.

Comments about the success of your search appear in the lower portion of the window. You can choose View Match List to display a list of matches instead. The View Match List button changes to the Search Expert button. To redisplay the comments, choose Search Expert.

7. Close the Search window by choosing Close.



In the OMNIC Help system Index, find “library, searching” and go to the “Searching a spectral library” topic for more information on searching spectral libraries.

Creating and printing a report

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

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 C:\OMNIC\REPORT directory and select the report template file named SEARCH1.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 for your report. You can view the image as a graphical layout by selecting the Layout option. This shows you how the printed report will look on paper. You can also view the image with template items labeled by selecting the Description option. This lets you identify items that are too small to be seen clearly.

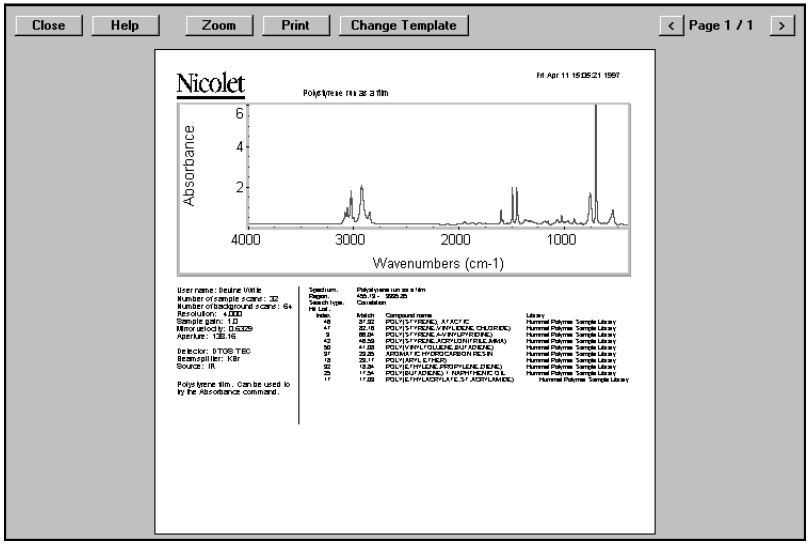
3. **Choose Select to make the example template the current template for printing reports.**

   When you print your report, OMNIC will automatically fill in the items in the template with the appropriate information and images. For example, if an item in the template is linked to the active spectral window, the contents of that window appear on paper 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 the OMNIC Help system Index, find "report template, selecting" and go to the "Selecting, editing or creating a report template" topic 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:



The preview lets you check the content of the report before printing it. Choose the Zoom button to see an enlarged image of the report.

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

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

6. **Choose OK.**

   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 the Add To Library button on the toolbar.**

   You can also 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 the OMNIC Help system Index, find "user library, adding a spectrum to" and go to the "Adding a spectrum to the user library" topic 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, QC library or scrapbook library.

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.

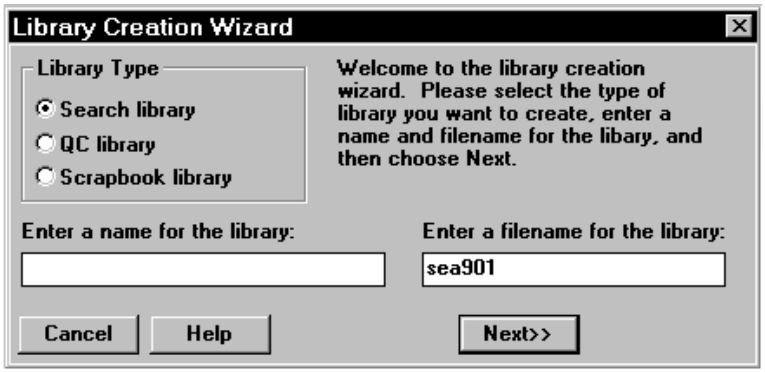
Once a library is created, you can add spectra to it with the Add To Library button (or with Add To Library in the Analyze menu) and use it just as you would a commercial library to identify unknown spectra or verify the composition of a sample. If you create a scrapbook library, you can find spectra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

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. For this example we will create a new search library.



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 your library listed by clicking the Search Libraries book on the Library Names tab.



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

Spectrometer Basics

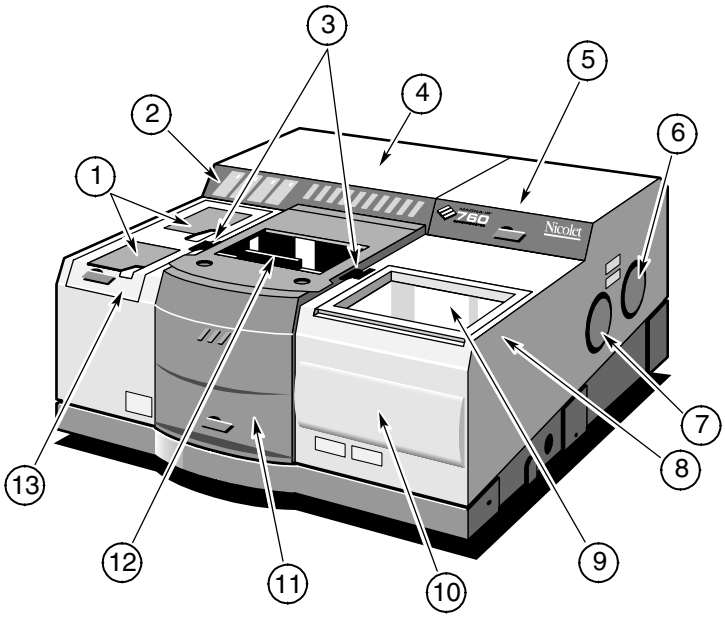
This chapter describes the major components of your spectrometer, including the light source, beamsplitter and detector. It then explains what you will need to know before collecting data in various spectral ranges.



View the “From the front,” “The back panel,” and “Inside the spectrometer” units of the “Spectrometer Tour” tutorial for complete descriptions of your spectrometer’s internal and external components.

Major spectrometer components

The following illustration and table identify the major components of the System 760 spectrometer. The System 560 is identical except that it has a single door for filling a detector dewar, in the front position, and does not have a detector access hatch* or beamsplitter compartment hatch.



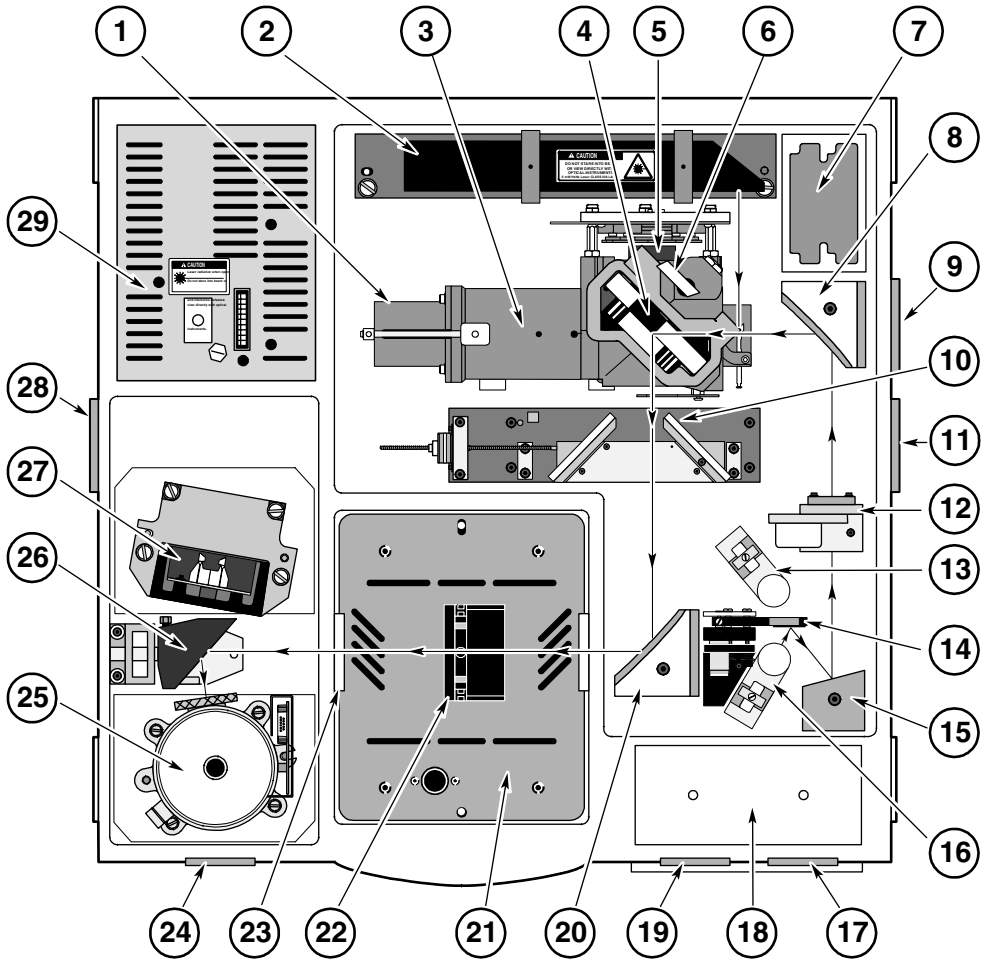
* The detector access hatch is available as an option on the System 560.

Number	*Description*
1	Access doors for filling the detector dewars with liquid nitrogen.
2	Front panel with Power, Scan, Laser and Source indicator lights.
3	Purge shutters for sealing off the sample compartment when you install a sample.
4	Electronics cover.
5	Beamsplitter compartment hatch.
6	Emission port for an external source.
7	External beam port.
8	Desiccant area (under the sample tray) for holding the desiccant (in sealed and desiccated systems only).
9	Sample tray for holding samples and other items needed for your experiments.
10	Beam ports (behind the snap-on cover) for special applications such as the integrated SabIR™ accessory.
11	Sample compartment cover.
12	Sample compartment sliding door for installing samples.
13	Detector compartment access hatch.

▲ **Caution** To avoid overheating of electronic components, do not place anything on top of the electronics cover of the spectrometer. ▲

What's inside?

The illustration below shows a top view of the optical layout of the System 560 or 760 spectrometer with covers removed to reveal components. See the table that follow for identifications of the numbered components. The dashed line containing arrows shows the path of the infrared beam.



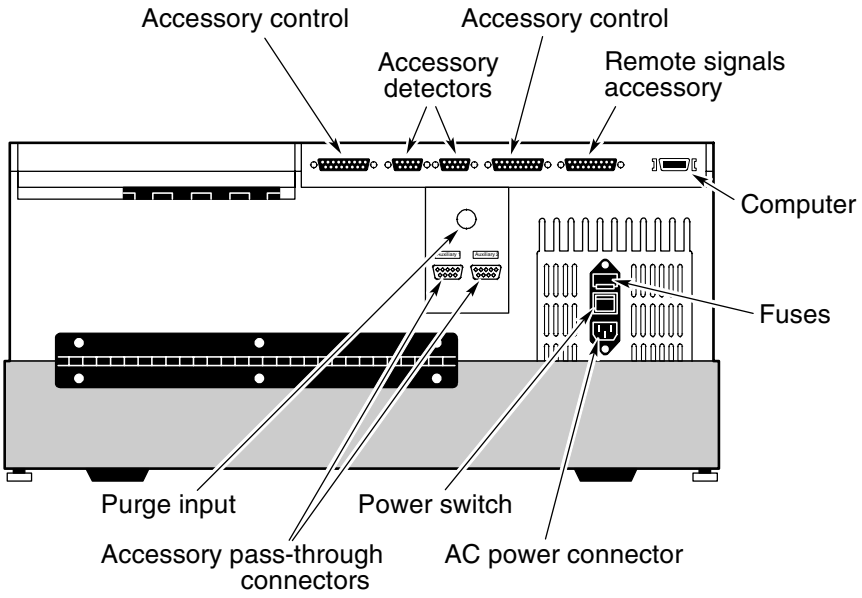
Number	*Description*	*Number*	*Description*
1	Interferometer	16	Near-IR source (optional; requires quartz or CaF_2 beamsplitter)
2	Laser	17	SabIR fiber optic detector port (optional)
3	Moving mirror	18	Special detector mounting pad
4	Beamsplitter	19	Seaport external beam port
5	Fixed mirror	20	Sample focus mirror
6	Beamsplitter latch	21	Sample compartment
7	Beamsplitter storage area	22	Sample holder
8	Parabolic mirror or optional Import emission optics	23	Energy screen or filter (optional)
9	External emission source port	24	Optional port for far-IR bolometer detector
10	Passport optics (optional)	25	Front detector location
11	Right-side external beam port	26	Monoflect detector mirror
12	Aperture	27	Back detector location
13	Ever-Glo IR source	28	Left-side external beam port
14	Source selection mirror (optional)	29	Power supply
15	Source focus mirror		



View the “Inside the spectrometer” unit of the “Spectrometer Tour” tutorial for complete descriptions of your spectrometer components.

What is on the rear panel?

The following illustration shows the locations of the connectors, purge input, fuses and power switch on the spectrometer rear panel:

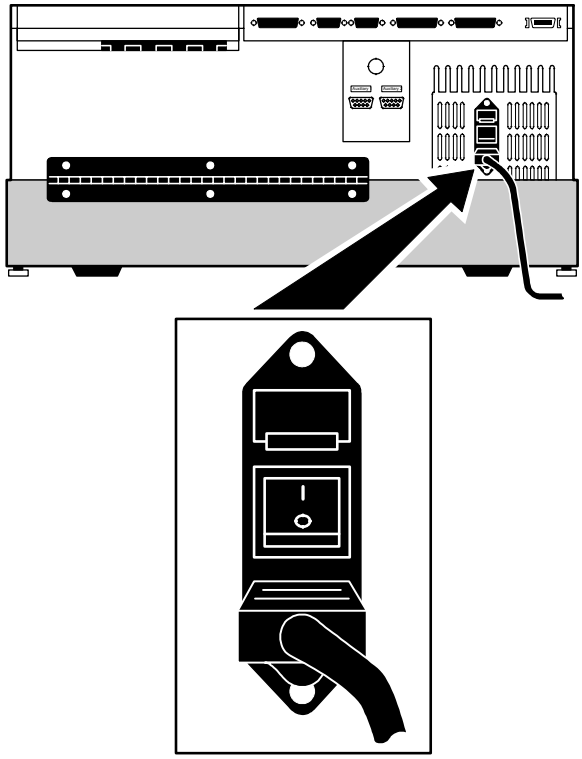


View “The back panel” unit of the “Spectrometer Tour” tutorial for complete descriptions the rear panel components.

For descriptions of the Accessory pass-through connectors, see the “How to cable an accessory” section of the “Accessories You Can Buy and How to Install Them” chapter of this manual.

Turning on the spectrometer power

To turn on the spectrometer, press the power switch (I/O) on the rear panel to I. To turn the spectrometer off, press the switch to O. The following illustration shows the location of the power switch:



⚠ Warning Do not operate the spectrometer without following the safety precautions described in this manual and in the *Optical Bench Safety Guide* that came with your system. ▲

View the "Powering Up" unit of the "Spectrometer Tour" tutorial for complete instructions on turning on your system.

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. ▲

▲ Caution To avoid overheating the electronic components, do not place anything on top of the electronics cover (left-rear cover) of the spectrometer. See the first illustration in this chapter for the location of the cover. ▲

When you turn on the spectrometer, the four indicators on the front panel—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 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 OMNIC screen. If you cannot resolve the problem, 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: 1-608-273-6045
- World Wide Web: http://www.nicolet.com
- E-mail: nicinfo@nicolet.com ▲

Using a light source

The System 560 and 760 spectrometers are available with a single internal source or with optional dual sources. If your spectrometer does not have the dual-source option, you will need to change sources in order to use a different internal source.



If you need to install or change a source, choose Replacing Parts from the OMNIC Help menu and view the "Changing a Source" tutorial in the "Replacing parts" book.

⚠ 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. ▲

If your spectrometer has the dual-source option, you can use a different internal source by simply changing the Source setting on the Bench tab of the Experiment Setup dialog box. This option lets you collect data in the mid-IR to far-IR range or in the visible to near-IR range. The spectral range is determined by the source you are using and by the selected detector and beamsplitter.

System 560 and 760 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 the OMNIC Help system Index, find "source" and go to the "Specifying the source type" topic for instructions on using different sources in spectrometers with single sources and with dual sources.

Using beamsplitters and detectors

A number of beamsplitters and detectors are available for use in the System 560 and 760. 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 chapter explains how to select and optimize the performance of beamsplitters and detectors.



If you need to install or change a beamsplitter or detector, choose Replacing Parts from the OMNIC Help menu and view the appropriate tutorial in the “Replacing parts” book.

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 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 beamsplitter and detector combination will provide the maximum capable sensitivity range of each component.

	BEAMSPLITTER					
		Near-IR		Mid-IR		Far-IR
DETECTOR	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

Best = Optimum beamsplitter-detector combination.
OK = Compatible beamsplitter-detector combination.
X = Incompatible beamsplitter-detector combination.

* Valid for room temperature and thermoelectrically cooled versions.

† These detectors are typically set up for optimum performance using a Gain setting of 4.

‡ Can be used only with the white light source.

§ Can be used only with the SabIR accessory.

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

Light Range	*Beamsplitter*	*Detector*	*Spectral Range (cm^{-1})*	*Source*
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
	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
	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
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
far-IR	Solid-Substrate	DTGS-PE	700 - 50	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

Magna-IR detectors can be optimized to produce a more linear response and greater photometric accuracy, or to increase the signal-to-noise ratio. These improvements in performance are each accomplished by adjusting the amount of infrared energy that reaches the detector.

Improving linearity and photometric accuracy

Some detectors (including Si, PbSe, 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, when compared with much larger background signals, can distort quantitative data.

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

To solve these problems, Magna-IR spectrometers allow the following options for modifying the infrared beam:

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



See “Setting up for experiments” available through Installing Hardware in the Help menu for instructions on installing filters and energy screens. In the OMNIC Help system Index, find “aperture” and go to the “Setting the aperture size” topic for information on changing the aperture setting.

In most cases, system performance will be better if you use a filter or screen instead of reducing the aperture size. 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

Nicolet offers several optional bandwidth-limiting filters for optimizing performance in the spectral range that they pass. These filters 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.

The following table lists the bandwidth-limiting filters available from Nicolet and indicates the band of energy that each filter passes. (Filters from other manufacturers that have the same optical characteristics can be used instead.)

Filter	*Band Passed by Filter*	*Typical Use*
polyethylene	700 - 50 cm^{-1}	far-IR
red	16,000 - 9,000 cm^{-1}	near-IR
broad-band blue	23,000 - 16,000 cm^{-1}	visible
narrow-band blue	26,000 - 21,000 cm^{-1}	visible



See “Setting up for experiments” available through Installing Hardware in the Help menu 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. In most cases system performance will be better if you use an energy screen instead of reducing the aperture size.

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

Screen	*% Transmitted**	*Detectors Typically Used With Screen*
none	100	DTGS, MCT-B
A	30	MCT-A, InSb
B	10	Si, PbSe
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.



See “Setting up for experiments” available through Installing Hardware in the Help menu for instructions on installing energy screens.

What aperture size to use for your detector

The aperture is a variable-diameter opening which controls the angular size of the infrared beam and, thus, the amount of radiation that reaches the sample. Using an aperture provides the following 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 Magna-IR 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 size of 8 mm and an approximate area of 0.50 cm^2. ▲

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 signal-to-noise ratio.

Detector	*Aperture Setting*
DTGS	100
MCT-A, MCT-B, InSb, PbSe, Si	32



In the OMNIC Help system Index, find “aperture” and go to the “Setting the aperture size” topic 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).

Other methods can be used with sensitive detector types. These include using an energy screen that transmits more light (or no screen at all) or increasing the aperture setting. With either of these corrections, 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. ▲



See "Setting up for experiments" available through Installing Hardware in the Help menu 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 the OMNIC Help system Index, find "aperture" and go to the "Setting the aperture size" topic 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.

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

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



See “Setting up for experiments” available through Installing Hardware in the Help menu for instructions on installing filters.

About the moving mirror velocity

While a wide range of moving mirror velocities is available on the System 560 and 760, some velocity settings cannot be used for collecting data at certain combinations of spectral range and resolution:

- If you are collecting data over a spectral range below 7899 cm^{-1} and at a resolution better than 2.0 cm^{-1}, do not use a velocity faster than 5.06 cm/sec.

- If you are collecting data over a spectral range above 7899 cm^{-1}, do not use a velocity faster than 2.53 cm/sec.

To specify the velocity and spectral range, use the Velocity and Spectral Range settings on the Bench tab in the Experiment Setup dialog box. To specify the resolution, use the Resolution setting 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 window. Be sure to check the range and set the velocity to a value that is appropriate (see the limitations described above). ▲

Accessories You Can Buy and How to Install Them

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.

Sampling accessories for different applications

You can install many of the 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, liquid analysis systems, and SabIR fiber optics with the System 560 and 760. A Raman accessory is also available for the System 760.

Some accessories have their own optics. The optional Passport optics inside the spectrometer redirect the light beam from the internal light source through a port on the right or left side of the spectrometer. The beam then travels into the accessory's optics. The Seaport option redirects the IR beam from the sample compartment to the front port position.

The collimated light beam from an accessory that includes its own external source can be directed into the System 560 or 760 optics through a port on the right side or front of the spectrometer. Using the port on the right side of the spectrometer requires a detector in the front or back detector location. Using the port on the front of the spectrometer requires an optional emission detector in the front-right detector location below the sample tray.



Some of the accessories fit into the sample compartment and require that you remove the standard Snap-In baseplate before installing the accessory. For instructions on using Snap-In baseplates, choose Replacing Parts from the OMNIC Help menu. Then choose the "Removing the snap-in baseplate" topic from the "Replacing parts" book.

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. ▲

ATR needle probe and FiberLink™ – 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 FiberLink 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.

Attenuated total reflection (ATR) – Attenuated total reflection accessories are used to sample highly absorbent solid and liquid materials, including surface films, coatings, polymers, powders and adhesives. These accessories can be installed in the main spectrometer sample compartment or in an auxiliary experiment module (AEM).

Attenuated total reflection kit (The A.R.K.™) – The A.R.K. 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.

The A.R.K. is also available as an E.S.P. accessory. E.S.P. accessories are automatically recognized by the Magna-IR E.S.P. spectrometer and OMNIC E.S.P. software. The system automatically selects the correct operating parameters for the system when the A.R.K. E.S.P. is installed. Also, a series of spectral quality checks are performed to ensure that the accessory is installed and operating correctly.



For instructions on installing E.S.P. accessories, choose Replacing Parts from the OMNIC Help menu. Then choose the "Installing optional hardware" topic from the "Replacing parts" book.

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 auxiliary experiment module (AEM) provides you with an additional sample compartment. The AEM can be positioned on either 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.

Detector interface kit – A variety of accessories (that were specifically designed for Protégé 460 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.

Diffuse reflection – 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. Diffuse reflection accessories can be installed in the spectrometer sample compartment or AEM.

Fiber optics – The SabIR fiber optic 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 and is available in versions that can be mounted in the sample compartment or in the front-right detector location below the sample tray. Mid-IR fiber optic accessories are available for mounting in the sample compartment.

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.

IR 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.

Liquid analysis system – The Nicolet Liquid Analysis System lets you collect and process quantitative analysis data for liquid samples. The System uses the OMNIC Integra™ software, which contains methods designed for quantifying components in specific types of liquids. The System can include a Programmable Liquid Uptake System (PLUS™) and an autosampler for automating liquid sample handling.

ProfilIR® – This accessory lets you perform automated, variable-angle, attenuated total reflection and external reflection experiments. Special cabling is required.

Raman – The Raman accessory can be attached to the right side of a Magna-IR 760 spectrometer and used with Nicolet's OMNIC For Raman software to collect and process FT-Raman spectral data. The accessory includes an excitation laser and a sample compartment. Several sampling configurations are available.

Start accessory – The Start 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.

Single Bounce Horizontal ATR (SB-HATR) – The SB-HATR accessory has a shorter pathlength and higher throughput than traditional horizontal ATR 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.

The SB-HATR is also available as an E.S.P. accessory. E.S.P. accessories are automatically recognized by the Magna-IR E.S.P. spectrometer and OMNIC E.S.P. software. The system automatically selects the correct operating parameters for the system when the SB-HATR E.S.P. is installed. Also, a series of spectral quality checks are performed to ensure that the accessory is installed and operating correctly.



For instructions on installing E.S.P. accessories, choose Replacing Parts from the OMNIC Help menu. Then choose the "Installing optional hardware" topic from the "Replacing parts" book.

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 then 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 – 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.

The standard transmission baseplate is also available as an E.S.P. accessory. E.S.P. accessories are automatically recognized by the Magna-IR E.S.P. spectrometer and OMNIC E.S.P. software. The system automatically selects the correct operating parameters for the system when the Transmission E.S.P. baseplate is installed. Also, a series of spectral quality checks are performed to ensure that the baseplate is installed and operating correctly.

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.

RSVP Remote diagnostics – This option uses a data modem and remote control software to allow control of your computer (and spectrometer) through the modem link. An analog telephone line is required.

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.

Using pass-through connectors

Your spectrometer is 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.

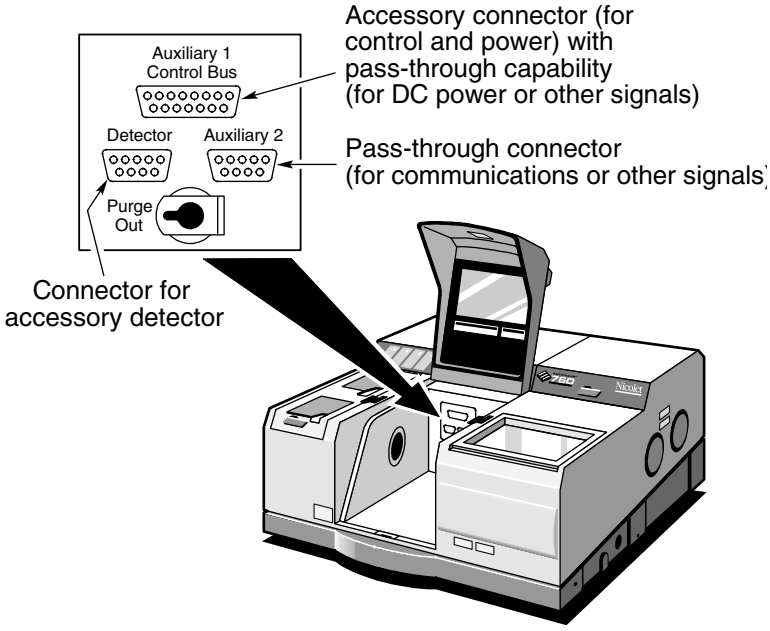
⚠ Warning Improper or unsafe cabling can cause damage to your accessory and may create a safety hazard. Only qualified persons should cable a custom accessory using these connectors. Nicolet is not responsible for damage or injury resulting from improper or unsafe cabling. ▲

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.

Note The "Using connectors for custom accessories" section later in this chapter contains current, voltage, pin connection and other limitations on using these connectors. ▲

Connectors inside the sample compartment

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



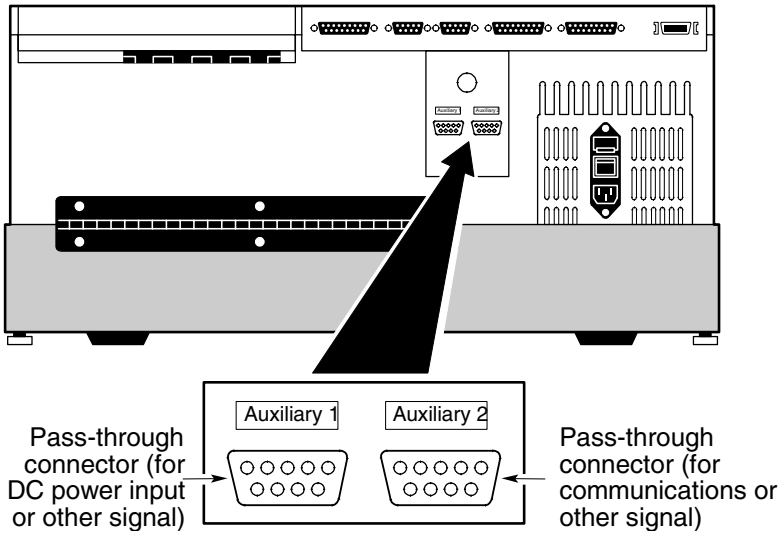
Auxiliary 1/Control Bus – Seven pins on this connector are used to provide power and communications between the spectrometer and an accessory. Accessories such as the Nicolet sample shuttle use this capability. Nine pins on the connector can be used for passing DC power input or other signals from the Auxiliary 1 connector 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.

Detector – If you have a photoacoustic or other accessory that has a detector located in the spectrometer sample compartment, connect the cable from the detector to this standard connector.

Auxiliary 2 – This connector can be used for passing communications or other signals from the Auxiliary 2 connector on the rear panel. For example, you can use this connector to attach the communications cable from the automatic sample wheel or the ProfilIR accessory.

Connectors on the rear panel

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



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

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

Using connectors for custom accessories

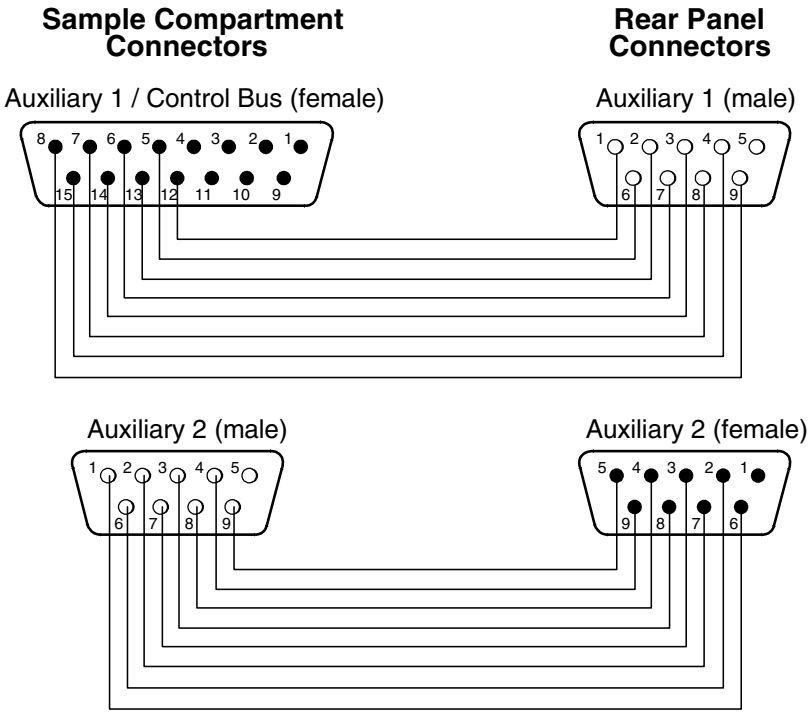
You can use the pass-through connectors to provide power and communication or other signals for your own custom accessories.

⚠ 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. ▲

By connecting custom cables that use these pins, you can pass power and one or more signals through the spectrometer from the rear panel to the sample compartment and vice versa, so long as the voltage does not exceed ±15 VDC and you limit the current to a maximum of 800 mA.

▲ Caution When designing a cable to be used on the Auxiliary 1 connector in the sample compartment, *never* connect signals to pins 1 through 4 and pins 9 through 11. These pins carry DC power, ground and communications signals from the spectrometer. They are not available for use with custom accessories. Connecting these pins could damage your accessory or the spectrometer. ▲

The following diagram shows schematically, with solid lines, which pins of the connectors inside the sample compartment are *internally* connected to pins of the connectors on the rear panel. Since none of these connected pins are assigned by the Magna-IR system, they are available for use with custom accessories.



Quick Answers to Your Questions About Using OMNIC E.S.P.

This chapter presents common questions and answers about using the OMNIC software. Each question is followed by a brief answer, plus a reference for where you can 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.



View the "Preparing the Software" unit of the "Collecting a Spectrum" tutorial for information on setting the software for collecting spectra.

In the OMNIC Help system Index, find "selecting, experiment" and go to the "Selecting an experiment" topic, or find "experiment, parameters" and go to the "Setting the experiment parameters" topic.

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.



View the "Collecting the Spectrum of a Sample" unit of the "Collecting a Spectrum" tutorial for information on collecting spectra.

In the OMNIC Help system Index, find "collecting, spectrum" and go to the "Collecting a sample spectrum" topic or "Collecting a background spectrum" topic.

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.



View the "Typical IR Transmission Spectrum" unit of the "Collecting a Spectrum" tutorial.

In the OMNIC Help system Index, find "Y-axis, unit" and go to the "Selecting a final format" topic.

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.



View the "Setting the Instrument Gain" unit of the "Collecting a Spectrum" tutorial.

In the OMNIC Help system Index, find "gain" and go to the "Setting the gain" topic.

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.



View the "Setting parameters for automatic saving" lesson of the "Preparing the Software" unit of the "Collecting a Spectrum" tutorial.

In the OMNIC Help system Index, find "saving, interferograms" and go to the "File handling" topic.

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.



View the “Collecting the Spectrum of a Sample” unit of the “Collecting a Spectrum” tutorial.

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.



In the OMNIC Help system Index, find “quality” and go to the “Quality tab” topic.

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 sampling 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.



View the “Typical IR Transmission Spectrum” unit of the “Collecting a Spectrum” tutorial.

In the OMNIC Help system Index...

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

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

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

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

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

Find “log (1/R) units” and go to the “Log (1/R) units” topic.

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 choosing Search from the Analyze menu.



In the OMNIC Help system Index, find "searching, spectral library" and go to the "Setting up a library search" topic or "Searching a spectral library" topic.

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 the OMNIC Help system Index, find "correcting, baseline" and go to the "Correcting a baseline manually" topic.

- 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 the OMNIC Help system Index, find "blanking spectral region" and go to the "Blanking a spectral region" topic.

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 the OMNIC Help system Index, find “selecting, spectral region” and go to the “Region tool” topic, or find “displaying, spectral region” and go to the “View finder” topic.

- 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 the OMNIC Help system Index, find “Kramers-Kronig transformation” and go to the “Kramers-Kronig (dispersion) transformation” topic.

- 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.



View the “Using an ATR Accessory” tutorial for information on using your ATR. In the OMNIC Help system Index, find “ATR correction” and go to the “ATR correction” topic.

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



In the OMNIC Help system Index, find “water” and go to the “H2O and CO2 correction” topic.

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 the OMNIC Help system Index, find "selecting, spectral region" and go to the "Region tool" topic, or find "displaying, spectral region" and go to the "View finder" topic.

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. You can also double-click a spectrum on the Library Spectra tab.

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 or 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 the OMNIC Help system Index, find "user library, creating" and go to the "Creating a user library" topic.

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 the Library Manager and choose a spectrum.



In the OMNIC Help system Index, find “displaying, library spectrum” and go to the “Working with libraries” topic.

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 the OMNIC Help system Index, find “searching, spectral library” and go to the “Searching a library for text” topic.

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 the OMNIC Help system Index, find “extended search” and go to the “Using extended search” topic.

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 the OMNIC Help system Index, find "collecting, spectrum" and go to the "Working with libraries" topic.

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 (or click the Open button in the toolbar if displayed), locate the spectrum or spectra you want to open, select the filenames of the spectra and then choose OK. You can also hold down the Control key and select multiple files to open.



In the OMNIC Help system Index, find "opening, spectrum" and go to the "Opening spectra" topic.

How can I automatically save my collected spectra?

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.



View the "Setting parameters for automatic saving" lesson in the "Preparing the Software" unit of the "Collecting a Spectrum" tutorial.

In the OMNIC Help system Index, find "saving, spectra" and go to the "File handling" topic.

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 the OMNIC Help system Index, find "report notebook" and go to the "Adding a report to a notebook" topic.

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 the OMNIC Help system Index, find "spectrum" and go to the "Adding a spectrum to a user library" topic.

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 the OMNIC Help system Index, find "spectrum, saving" and go to the "Saving spectra with a new filename" topic.

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 the OMNIC Help system Index, find "saving, spectra" and go to the "Saving a group of spectra" topic.

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 the OMNIC Help system Index, find “deleting, spectra” and go to the “Deleting files” topic.

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 subdirectory 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 the OMNIC Help system Index, find “printer” and go to the “Setting up the printer” topic.

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.



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

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 the OMNIC Help system Index, find “adding, report to notebook” and go to the “Adding a report to a notebook” topic.

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

Displaying spectra

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

Hold down the Control key while you click the spectrum. You can also choose Select All from the Edit menu to select all the spectra in the window that are not hidden.



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

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 the OMNIC Help system Index, find “spectra, colors” and go to the “Specifying colors for spectra and other features” topic.

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 the OMNIC Help system Index, find “spectra, colors” and go to the “Selecting a color for the currently selected spectra” topic.

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 the OMNIC Help system Index, find “display parameters” and go to the “Setting the display parameters” topic, or find “Window options” and go to the “Window options” topic.

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 system Index...

For information on Full Scale or Automatic Full Scale, find "displaying, spectra" and go to the "Displaying spectra full scale" topic or "Displaying spectra full scale automatically" topic.

For information on Common Scale, find "displaying, spectra" and go to the "Displaying spectra using the same Y-axis" topic.

For information on Match Scale, find "displaying, spectra" and go to the "Matching the Y scale of a spectrum" topic.

For information on Offset Scale, find "displaying, spectra" and go to the "Displaying spectra vertically offset" topic.

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 the OMNIC Help system Index, find "expanding, spectrum" and go to the "Selection tool" topic, "View finder" topic or "Rolling and zooming spectra" topic.

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 the OMNIC Help system Index, find "moving, spectrum" and go to the "Selection tool" topic or "Rolling and zooming spectra" topic.

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 the OMNIC Help system Index, find "moving, spectrum" and go to the "Selection tool" topic, or find "pasting, spectrum" and go to the "Pasting items" topic.

How can I move a stacked spectrum into another pane?



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



In the OMNIC Help system Index, find "moving, spectrum" and go to the "Selection tool" topic.

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 the OMNIC Help system Index, find “Displaying, X and Y values” and go to the “Spectral cursor tool” topic.

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 the OMNIC Help system Index, find “Peak, height” and go to the “Peak height tool” topic.

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 the OMNIC Help system Index, find “Peak, area” and go to the “Peak area tool” topic.

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.



View the “Common Problems” unit of the “Collecting a Spectrum” tutorial.

In the OMNIC Help system Index, find “correcting, baseline” and go to the “Correcting a baseline manually” topic.

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 in the Process menu 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 the OMNIC Help system Index, find “subtracting, spectra” and go to the “Subtracting spectra” topic.

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 arithmetic operations can I perform on my spectra?

You can manipulate your spectra using any of the common arithmetic 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.



In the OMNIC Help system Index, find “spectrum” and click the topic that corresponds to the operation you want to perform.

Customizing OMNIC

How can I customize my OMNIC software?

You can use Options in the Edit menu to set options that determine how the software operates. You can also customize the menus and the toolbar using Edit Menu and Edit Toolbar in the Edit menu. Use Save Configuration As in the File menu to save your customized settings in a configuration file. You can then open the file later to reset OMNIC to your preferences in one step.



View the “Preparing the Software” unit of the “Collecting a Spectrum” tutorial.

In the OMNIC Help system Index...

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

Find “customizing, menu” and go to the “Customizing a menu” topic.

Find “customizing, toolbar” and go to the “Customizing a toolbar” topic.

Find “saving, configuration” and go to the “Saving a configuration” topic.

Find “opening, configuration” and go to the “Opening a configuration” topic.

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.

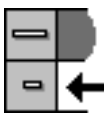


In the OMNIC Help system Index, find “finding peaks” and go to the “Finding peaks above a specified height” topic, or find “labeling peaks” and go to the “Annotation tool” topic.

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



In Windows 95 or Windows NT 4.0, click the Close button (if available) in the upper-right corner of the window or 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 Windows 3.1 (or 3.11) or Windows NT 3.5, double-click the Control-menu box in the upper-left corner of the task window (**not** the OMNIC window’s Control-menu box).





In the OMNIC Help system Index, find “closing, task window” and go to the “Task windows” topic.

How can I select a spectral region for an operation?



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



In the OMNIC Help system Index, find “selecting, spectral region” and go to the “Region tool” topic.

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 the OMNIC Help system Index, find "collection and processing information" and go to the "Collection and processing information" topic.

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 the OMNIC Help system Index, find "displaying, sampling information" and go to the "Displaying sampling information" topic.

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 the OMNIC Help system Index, find "copying, spectrum" and go to the "Copying items" topic.

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.

What telephone number should I call to get answers to other questions?

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: 1-608-273-6045
- World Wide Web: http://www.nicolet.com
- E-mail: nicinfo@nicolet.com ▲

Quick Answers to Your Questions About Using the Spectrometer

This chapter presents common questions and answers about using your spectrometer. Each question is followed by a brief answer, plus a reference for where you can 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 Si, PbSe, 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.



See “Setting up for experiments” available through Installing Hardware in the Help menu for instructions on installing energy screens.

Do I need to use a bandwidth-limiting filter?

If you are using a highly sensitive detector such as a Si, PbSe, MCT-A or InSb detector and your experiment deals with information in a narrow range of frequencies, a bandwidth-limiting filter can prevent the detector from becoming saturated or producing a distorted signal. Bandwidth-limiting filters 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.



See “Setting up for experiments” available through Installing Hardware in the Help menu for instructions on installing filters.

Why do I need to use an aperture?

An aperture of the appropriate size is needed to preserve the line shape of spectra when you collect data at higher resolutions. OMNIC automatically calculates the default aperture size based on the resolution, mirror velocity and spectral range. If you change the settings of these items, the software changes the aperture setting accordingly and informs you when you close the Experiment Setup dialog box. You can then specify whether to use the changed setting or the previous setting.



In the OMNIC Help system Index, find "aperture" and go to the "Setting the aperture size" topic for information on setting the Aperture parameter.

When do I need to open the spectrometer cover?

If you have a System 560, you need to open the spectrometer cover to change beamsplitters or detectors. Also, you need to open the cover of a System 560 or 760 if you are installing a spectrometer component such as a source, laser or power supply.



See "Opening the cover" available through Replacing Parts in the Help menu for instructions on opening the cover.

⚠ 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.



View the “Testing Performance” unit of the “Collecting a Spectrum” tutorial for information on when to align the spectrometer.

In the OMNIC Help system Index, find “aligning, optical bench” and go to the “Aligning the optical bench” topic for information on performing an automatic alignment.

Does my detector need to be cooled with liquid nitrogen?

Detectors that have a dewar need to be cooled. Dewar detectors are fairly large silver cylinders with a hole in the top. These include MCT and InSb detectors. To determine if your detector requires cooling, open the detector access door, or the spectrometer cover if there is no access door, 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.



Choose Replacing Parts from the OMNIC Help menu and view the “Cooling a detector” tutorial in the “Replacing parts” book for information on cooling a detector.

When should I change the desiccant?

If your spectrometer is sealed and desiccated, there is an indicator in the optics area that shows when the desiccant needs to be changed. You should check the indicator every two months. To check the indicator, remove the sample tray from the main cover of the spectrometer. If the indicator is pink, the desiccant needs to be replaced. The indicator itself does not need to be replaced.

See the replacement parts list included in your manual set to find the part number for desiccant packets. Packets come in sets of five, but four packets should be enough for replacement.



Choose Replacing Parts from the OMNIC Help menu and view the "Changing desiccant" tutorial in the "Replacing parts" book for information on checking and changing the desiccant.

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 the OMNIC Help system Index, find "source" and go to the "Specifying the source type" topic for information on setting the Source parameter.

See "Selecting the right beamsplitter and detector" in the "Using beamsplitters and detectors" section of the "Spectrometer Basics" chapter of this manual for a table showing the compatibility of sources, beamsplitters and detectors.

What do the purge shutters do?

When closed, the purge shutters seal off the optics areas of the spectrometer from the sample compartment. This allows you to open the sample compartment to install a sample or accessory without letting water and carbon dioxide enter the rest of the spectrometer.



View the "Purging the optical bench" lesson in the "Preparing Your Optical Bench" unit of the "Collecting a Spectrum" tutorial for information on connecting using the purge shutters.

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 displays on your screen.



See the troubleshooting information available through Troubleshooting in the Help menu for instructions on diagnosing spectrometer problems, ordering parts and replacing parts.

Note If you wish 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. See the "Service and Maintenance" chapter of this manual for more information.



In the OMNIC Help system Index, find "diagnostics" and go to the "Checking bench components" topic.

How do I replace parts in the spectrometer?



Choose Replacing Parts from the OMNIC Help menu and choose the appropriate part.

What telephone number should I call to get answers to other questions?

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: 1-608-273-6045
- World Wide Web: http://www.nicolet.com
- E-mail: nicinfo@nicolet.com ▲

Service and Maintenance

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

⚠ Warning Perform *only* those routines 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: 1-608-273-6045
- World Wide Web: http://www.nicolet.com
- E-mail: nicinfo@nicolet.com ▲



See the troubleshooting information available through Troubleshooting in the Help menu for instructions on diagnosing spectrometer problems, ordering parts and replacing parts.

Running diagnostic tests

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. You should run these diagnostic tests if you have problems with your spectrometer to determine the source of the problem.

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.**

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 see information about a component, click that component's indicator icon.**

   When you click one of the indicators, a dialog box appears showing information about 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.

Service

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. See the troubleshooting information available through Troubleshooting in the Help menu for instructions on diagnosing spectrometer problems, ordering parts and replacing parts. ▲

If the source, laser module or power supply must be replaced, refer to the replacement parts list available through Replacing Parts in 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., contact your local Nicolet office. Telephone numbers for all Nicolet Customer Support offices are provided with your system.

Maintenance

The rest of this chapter describes how to use the OMNIC software to align the spectrometer and accessories, and run performance tests.



Instructions for other common maintenance procedures, such as changing desiccant, cleaning the purge filter and cleaning the outside of the spectrometer are available on-line. Choose the "Maintaining your optical bench" book available through Replacing Parts in the Help menu.

Alignment

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

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

Follow these steps:

1. **Remove any sample or accessory from the spectrometer.**

   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 a value that is appropriate for the detector type you are using. Do not use Autogain.**

   An interferogram is shown in the live display. In the OMNIC Help system Index, find "experiment" and go to the "Using Experiment Setup" topic for more information.

   If you want to view a single-beam spectrum instead, turn on the Single Beam check box on the Bench tab.

   If you want to hear a tone whose pitch indicates the signal intensity, turn on the Tone check box on the Bench tab. 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 IR 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 highest and lowest signal intensities are shown next to Max and Min at the top of 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, 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.

Performance test

The performance test can be used 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 to conduct a performance test:

1. **Make sure the main sample compartment is empty.**

   Remove any samples and sampling accessories.

2. **Exit OMNIC to ensure that the Bench Diagnostics software runs correctly.**

3. **Start the Bench Diagnostics software.**

   Click the Start button, then the Programs icon and then the OMNIC folder. Choose Bench Diagnostics.

   For more information on running the Bench Diagnostics programs, see the "Bench Diagnostics" section in the "Troubleshooting Hardware Problems" chapter of this manual.

4. **Follow the directions that appear on the screen to run the performance test.**

   Click the Performance Tests button and conduct the test as instructed by the software.

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., call your local service representative. Telephone numbers for all Nicolet Customer Support offices are provided with OMNIC Help. ▲

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.

Troubleshooting Software Problems

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

This chapter lists some simple troubleshooting measures you can take to solve software problems with the OMNIC software. If the action does not solve the problem, call your Nicolet service office.

Note For more information on troubleshooting, consult the OMNIC on-line Help system. ▲

Problem	Possible Cause	Solution
After data collection a message says the sample and background spectra have the wrong resolution.	The resolution or data spacing of the current background spectrum does not match the resolution selected for the sample spectrum collection.	Change the setting of Resolution to a value within the specified range and collect the spectrum again.
The Quantify command is dimmed.	No quantitative analysis method is selected. No spectrum is selected. The quantitative analysis Quantify method is not appropriate for the selected spectrum.	Select the quantitative analysis method using Quant Setup in the Analyze menu. Select a single spectrum. Select an appropriate method for the selected spectrum.
OMNIC needs to be restored after a system crash or a 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 OMNIC. Run the SCANDISK utility included with your Windows software. Reinstall the OMNIC software.

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.

This chapter lists some simple troubleshooting measures you can take to solve problems with the spectrometer. The Bench Diagnostics program is described at the end of the chapter. If your actions do not solve the problem, call your Nicolet service office.

Note For more information on troubleshooting, use Troubleshooting in the OMNIC Help menu. ▲

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

Problem	Possible Cause	Solution
The indicators on the front panel do not light when the spectrometer is turned on.	The spectrometer is not plugged in.	Make sure the power cord is plugged into the spectrometer and a working wall outlet.
	The power cable or power supply is defective.	Call Nicolet to order a replacement part.
	A fuse is blown.	Replace the fuse. Choose Replacing Parts from the OMNIC Help menu and choose the "Replacing a fuse" tutorial from the "Replacing parts" book.
The Scan indicator on the front panel does not flash (the system is not scanning).	The spectrometer is out of alignment.	Align the spectrometer. Use the Align button on the Diagnostic tab in the Experiment Setup dialog box.
	After 1 hour without data collection activity, the interferometer stops scanning and the Scan light stays on. This mode is normal.	No action is required. Any data collection activity will cause the interferometer to begin scanning.
	The beamsplitter is not properly seated.	Check the beamsplitter.
	The spectrometer cover is ajar.	Close the cover and tighten the cover thumbscrews.
	An electronic miscue has occurred.	Turn off the spectrometer power for 10 seconds.
	A component has failed.	Call Nicolet for service.
There is frost on the outside of the detector.	The insulating vacuum chamber surrounding the dewar has begun to leak.	If you suspect that your detector has a vacuum leak, choose Troubleshooting from the OMNIC Help menu.

Problem	Possible Cause	Solution
Data are not displayed during data collection.	The laser is not functioning.	Hold a business card or other small piece of white paper in the beam path in the sample compartment to check for laser light. Replace the laser if necessary.
	The data cable between the spectrometer and computer is not properly connected.	Turn the spectrometer power off and check the data cable connections.
The Source indicator on the front panel is off.	The source is burned out.	Call Nicolet to order a replacement source. Choose Replacing Parts from the OMNIC Help menu and the "Replacing a source" tutorial from the "Replacing parts" book to find the part number, ordering and installation instructions.
The system does not scan.	The laser is flickering.	Hold a business card or other small piece of white paper in the beam path in the sample compartment to see if the laser light flickers. If it does, call Nicolet for service.
The signal intensity is low, there are frequent modulator scan restarts (verified by intermittent flashing of the Scan indicator) and the spectrometer alignment fails.	The beamsplitter is fogged.	Check the laser signals by clicking the laser indicator on the Diagnostic tab in the Experiment Setup dialog box, remove the beamsplitter and check the beamsplitter center window for fogging (check the clear area located in the center of the substrate). Replace the beamsplitter if necessary.
The signal intensity is low in the mid-IR range.	The source is glowing unevenly.	Check to see if the source element is glowing evenly. Order a replacement if needed.

Problem	Possible Cause	Solution
An error message appears when you try to scan.	The light source is not working.	Check the Source indicator on the front panel. If the light is out, replace the source.
	The detector is not cooled.	Check and cool the detector.
	The interferogram is not located at 1024 ±16 data points on the Bench tab in the Experiment Setup dialog box.	Align the spectrometer. If the interferogram is still not located correctly, call Nicolet for service.
	The beam path is blocked.	Hold a business card or other small piece of white paper in the beam path in the sample compartment to check for laser light. If no laser light is visible the beam path may be blocked. Remove the obstruction.
	The data cable between the spectrometer and computer is not properly connected.	Turn off the spectrometer power and check the data cable connections.
	The detector and beamsplitter are not compatible.	Change the detector or beamsplitter.
You encounter problems when selecting external detectors on a Nicolet AEM, GC interface or microscope.	A custom detector is selected on the Bench tab of the Experiment Setup dialog box.	Change the Detector setting to None on the Bench tab of the Experiment Setup dialog box.
	A detector cable is loose at the accessory connector (on the rear of the spectrometer or on the back wall of the sample compartment).	Check and tighten the cables.

Problem	Possible Cause	Solution
The baseline is not stable.	The purge rate is too high.	Lower the purge rate until the baseline is stable.
	The center laser detector is misaligned.	Use the Bench Diagnostics program to check the laser levels for proper balance. If the levels are out of tolerance, align the spectrometer using the Align button on the Diagnostic tab in the Experiment Setup dialog box. If the levels remain out of tolerance, call Nicolet for service.
	The desiccant is expired.	Replace the desiccant.
	The spectrometer cover was recently opened.	Allow the spectrometer to purge for 3 to 5 minutes after the cover is closed.
The Laser indicator on the front panel is off.	The spectrometer cover or beamsplitter compartment hatch (760 only) is not fully closed.	Turn off the spectrometer power, disconnect the power cord, and open the main cover. Make sure the DC power cable connecting the power supply to the bottom of the electronics printed circuit board (located in the raised spectrometer cover) is not pinched between the spectrometer cover and the power supply, preventing the spectrometer cover from seating properly. Make sure the beamsplitter compartment hatch (760 only) is fully closed.
	The laser is burned out.	Call Nicolet to order a replacement laser. Choose Replacing Parts from the OMNIC Help menu and the "Replacing the laser" tutorial to find the part number, ordering and installation instructions.

Problem	Possible Cause	Solution
The system scans but gives a very low signal intensity.	The spectrometer is out of alignment.	Align the spectrometer. Use the Align button on the Diagnostic tab in the Experiment Setup dialog box.
	The aperture setting is wrong.	Set the aperture to the proper setting.
	The detector and beamsplitter are not compatible.	Make sure that the selected detector and beamsplitter are compatible. Change the detector or beamsplitter if necessary.
	There is no interferogram.	If the Source indicator on the front panel is off, click the source indicator on the Diagnostic tab in the Experiment Setup dialog box to check the source current and voltage. If the Source indicator is on, check the interferogram on the Bench tab in the Experiment Setup dialog box; if the interferogram is not present, check the beam path and detector.

Bench Diagnostics

You can use the Bench Diagnostics program to perform diagnostic tests on the main components of the spectrometer. You should run these diagnostic 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.

You can use the Bench Diagnostics program 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 Bench Diagnostics:

1. **Make sure the main sample compartment is empty.**

   Remove any samples and sampling accessories.

2. **Start the Bench Diagnostics software.**

   Choose Advanced Diagnostics from the Collect menu, or click the Start button, and then choose the Bench Diagnostics icon in the OMNIC folder. Some of the advanced features of the program, 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 diagnostics.**

   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 program by clicking the Close button at the far right end of the title bar.

Troubleshooting Applications Problems

Your OMNIC 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.

Note For more information on troubleshooting, consult the OMNIC on-line Help system. ▲

Problem	Possible Cause	Solution
There are no peaks in a spectrum.	There is no sample in the path of the infrared beam.	Check the sample compartment or accessory to make sure the sample is properly positioned in the beam path.
	The sample and background spectra were collected with the purge shutters closed.	Open the purge shutters and collect the spectra again.
	The sampling cup in a diffuse reflection experiment is not in place or is tilted.	Make sure the cup is properly positioned in the diffuse reflection accessory.
	The infrared microscope is in its viewing mode.	Put the microscope in infrared mode and collect the spectrum again.
	The sample film in an attenuated total reflection (ATR) experiment is being held against the ATR crystal with uneven pressure or has poor contact with the crystal.	Make sure the sample is held evenly and has good contact with the crystal.
A spectrum contains totally absorbing peaks.	The sample in a transmission experiment is too thick.	Use a thinner sample.
A spectrum contains fringes or channeling.	A film sample may be too smooth.	Try roughening the film surface slightly with silicon carbide paper or another suitable abrasive.
	A film sample may be at the wrong angle with respect to the infrared beam.	Try positioning the sample at a different angle.

Problem	Possible Cause	Solution
A spectrum contains derivative-shaped peaks.	A sample in a diffuse reflection experiment also has a specular reflection component.	Correct the spectrum by using Other Corrections in the Process menu. (Select Kramers-Kronig.)
	The infrared beam was reflected from (instead of penetrating) a flat, shiny sample measured using a specular reflection accessory.	Try using a less reflective sample.
The baseline of a spectrum is not flat.	A KBr pellet was made with coarsely ground KBr powder, or the KBr pellet was improperly pressed.	Be sure to press the pellet properly.
	The background spectrum for a cast film was collected with an empty sample holder in the infrared beam.	Remove the sample holder and collect the background again.
	The spectrometer is not properly aligned, causing a sloped baseline.	Use the Align button on the Diagnostic tab in the Experiment Setup dialog box to align the spectrometer.
	The spectrometer has not been on long enough to reach thermal equilibrium.	For best results allow the spectrometer at least one hour to stabilize after turning it on.
	The spectrometer is not properly purged.	Check the system to make sure that the correct purge gas is being used and that the flow rate is correct.
A spectrum contains carbon dioxide peaks.	The spectrometer is not adequately purged.	Make sure you are using the correct purge gas and that the purge flow rate is adequate Allow the system three to five minutes to reestablish purge before collecting a spectrum.

Problem	Possible Cause	Solution
A spectrum contains water peaks.	The spectrometer is not adequately purged.	Make sure you are using the correct purge gas and that the purge flow rate is adequate. Allow the system three to five minutes to reestablish purge before collecting a spectrum.
	The desiccant has expired.	Check the desiccant and replace.
A spectrum is too noisy.	The detector is saturated.	Add bandwidth-limiting filters or energy screens to reduce signal strength.
	Too few scans.	Increase the number of scans on the Collect tab in the Experiment Setup dialog box.
	Too high resolution.	Reduce the resolution on the Collect tab in the Experiment Setup dialog box.

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