Thermo Nicolet

AVATAR®

User's Guide

For technical assistance, please contact:

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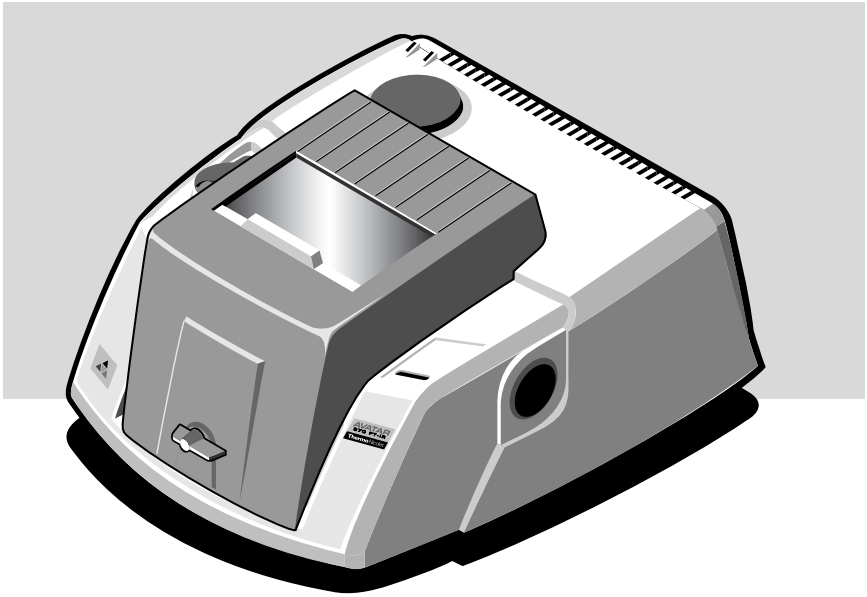
269-133800

Contents

Welcome!

Congratulations on your purchase of an Avatar® 330, 370 or 370 CsI spectrometer from Thermo Nicolet! Your Avatar system integrates advanced hardware features with the power and flexibility of Thermo Nicolet's OMNIC® or EZ OMNIC software*.



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

* Some dedicated systems use other Thermo Nicolet software packages.

About this manual

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

Depending on the model spectrometer you purchased, your system may include OMNIC, EZ OMNIC, or both. In this manual we will normally refer only to OMNIC and the OMNIC window. Except where indicated otherwise, the provided information also applies to EZ OMNIC and the EZ OMNIC window. See "If you are using EZ OMNIC" for more information about using that software.

This manual describes some hardware features that are not available on all Avatar models. Follow the instructions that apply to the features on your system.

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

This symbol tells you that you can find more information in the on-line tutorials. To access a tutorial, click the Help menu in OMNIC.

This symbol tells you that you can find more information in the on-line OMNIC Help system. Choose OMNIC Help Topics from the Help menu.

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

Note Notes contain helpful supplementary information.

(The symbol signifies the end of the Note, Caution, etc.)

Important Follow instructions labeled "Important" to avoid damaging the system hardware or losing data.

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

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

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

Questions and concerns

In case of emergency, if you have questions or concerns about safety or operating the spectrometer, or if you need assistance with repairs or replacement parts, contact Thermo Nicolet at the numbers listed below. If you are outside the U.S.A., call your local sales or service representative.

- Telephone (U.S.A.): 800-642-6538 or 608-276-6373
- Fax: 608-273-6883
- World Wide Web: http://www.thermo.com/nicolet
  (Choose ABOUT US and then click the desired location under "Contact Us" at the left side of the page.)
- E-mail: techinfo@thermonicolet.com

System requirements

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

- Intel® Pentium® II processor with 400 MHz clock speed.
- 128 megabytes of random access memory (RAM).
- Hard disk with 1.0 gigabyte of available space.
- Quad speed CD-ROM drive.
- 1.44-megabyte floppy disk drive for 3.5-inch floppy disks.
- 15-inch SVGA monitor with 800-by-600 resolution.
- 16-bit video card capable of displaying at least 256 colors with 1024 by 768 resolution.
- Sound card and speakers for listening to the audio portions of the tutorials.
- Keyboard and serial, bus, USB or PS/2®-style mouse.
- Parallel port for communication with the spectrometer.
- Printer port (USB, parallel and/or serial) if you plan to print on a local printer.
- Ethernet port if you plan to connect the system to a network.
- Internet connection if you plan to use the internet features of the software.
- An extra serial port if you plan to use a PLUS™ 2 Liquid Analysis System.
- Optical bench interface card and/or cable.
- Windows® 98, Windows NT® 4.0, Windows 2000, Windows Me or Windows XP.

Installing OMNIC

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

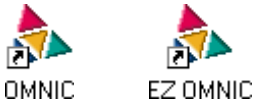
Starting OMNIC

Follow these steps to start OMNIC:

1. **Start your Windows software.**

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

2. **Double-click the OMNIC (or EZ OMNIC) shortcut on the Windows desktop.**



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

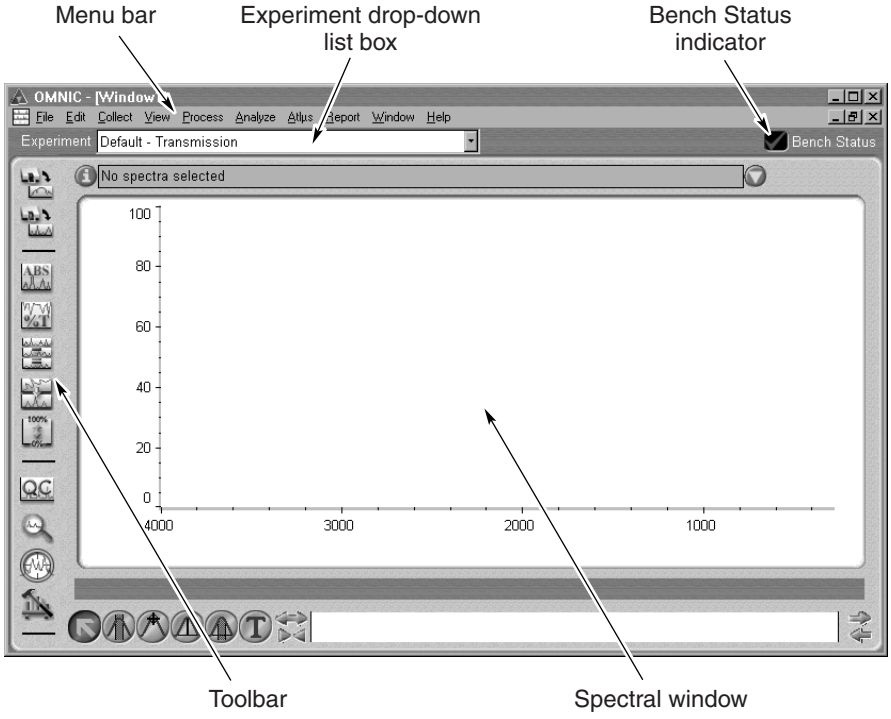
   Depending on how the program has been configured, dialog boxes may appear asking for a user name and password. Type the requested information and then choose OK.

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

The Avatar Installation Wizard may also appear. It contains instructions for installing your spectrometer and confirming its operation. You can turn off the wizard by clicking the check box on its last page. If you turn off the tutorial, you can still access it at any time by double-clicking the Avatar Installation Wizard shortcut on the Windows desktop.

The OMNIC window

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



Spectral window

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

Menu bar

Below the title bar is the menu bar, which contains all of the OMNIC menu names. (Depending on which optional software you purchased, the menu names in your menu bar may be somewhat different from those shown in the preceding illustration.) The menus are arranged in an order that you'll find convenient as you use the software. All of the menu commands are explained in detail in the on-line tutorials or the OMNIC Help system.

Experiment drop-down list box

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

Bench Status indicator

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

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

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

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

Toolbar

At the left side of the window is the toolbar. (You can use Edit Toolbar in the Edit menu to position the toolbar at the top or right side of the OMNIC window as well. In EZ OMNIC the default toolbar location is at the top.) Each button in the toolbar represents the action taken by a corresponding command or other feature. To see the name of the command or feature for a button, point to the button and wait a moment. To initiate the command or feature, click the button with the left mouse button.

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

Accessing on-line information

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 a variety of multimedia on-line tutorials, wizards and a complete Help system. These are described in the next sections

You can also find part numbers and hardware setup and replacement procedures when the computer is not connected to the spectrometer. In the Program Files\OMNIC folder, double-click the icon for the following programs:

Filename	*Description*
P370_ENU.HLP	Part numbers and hardware setup and replacement.
S370_ENU.EXE	Spectrometer tour.

Wizards and tutorials

The following wizards and tutorials are available on your system:

Avatar Installation Wizard – This wizard starts automatically whenever you start OMNIC and walks you step by step through installing your spectrometer and confirming that it is operating properly. Use the check box on the last page of the wizard after you have installed the spectrometer or if you do not want to see the wizard each time you start OMNIC. You can start this wizard at any time by double-clicking the Avatar Installation Wizard shortcut.

Getting Started With OMNIC – This tutorial, available through Getting Started in the Help menu, introduces you to OMNIC. It includes basic information about the OMNIC window, using the toolbar and tool palette, creating and using spectral libraries, creating your own experiment files, and using on-line laboratory notebooks to create and save reports. (The notebook and report features are not available in EZ OMNIC.)

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

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

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

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

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

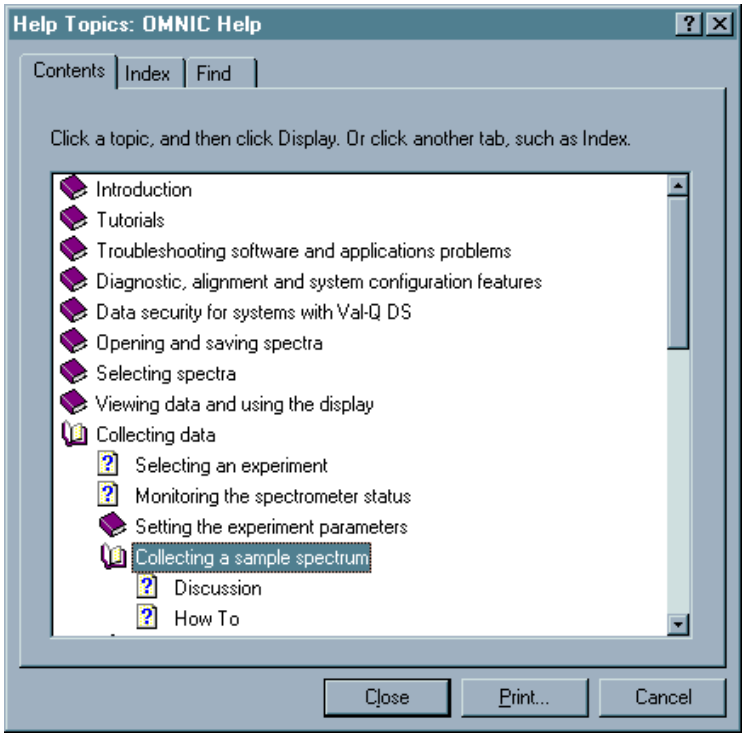
Technical Support – This tutorial, available in the Help menu, outlines the many support, training, and custom application services available from Thermo Nicolet. It includes Technical Support telephone and fax numbers, as well as e-mail and web site addresses.

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

OMNIC Help Topics

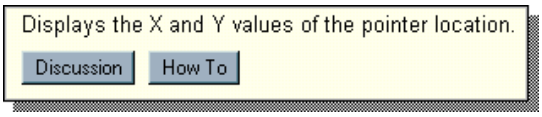
The OMNIC on-line Help system lets you quickly find answers to your questions about using the software.

To see the Contents of the Help system, choose OMNIC Help Topics from the Help menu. Here is an example of the Contents tab showing the contents of some of the books in the system:



There are several other ways to enter the Help system:

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



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

- You can press the F1 function key to see a discussion topic for the currently displayed or selected feature, dialog box or window.

- If a dialog box or window contains a Help button, click it to see information about the dialog box or window (or the command that displayed it).

If you are using EZ OMNIC...

The EZ OMNIC version of OMNIC includes the features you need to perform common spectroscopy tasks. If you are using EZ OMNIC, some of the features described in this manual are not available. Read and follow the instructions for the features that are in your software.

Here are some other things you should know about EZ OMNIC:

The **toolbar** is always displayed. It provides a convenient way to initiate menu commands, macros and external programs. For more information about the toolbar, find "toolbar" in the OMNIC Help system Index and go to the "Displaying and using a toolbar" topic.

You can use **Edit Toolbar** in the Edit menu to add available menu commands, macros, DDE commands or other programs. You can also specify the size of the toolbar buttons and whether text or icons, or both, appear on the buttons. For details, find "toolbar" in the OMNIC Help system Index and go to the "How to customize a toolbar" topic.

The **Search Method tab** appears in the Library Setup dialog box to allow you to specify a library search method. If you select Use Search Expert, the search expert determines the search algorithm to use for the best result and always searches the spectral region from 2600 to 450 wavenumbers. If you select Use Correlation Search, the correlation search algorithm is used for the search, and the search is performed over the full spectral range. For more information about the search expert, find "search expert" in the OMNIC Help system Index and go to the "Specifying the search results" topic.

A special command called **Create Library** appears in the Analyze menu to allow you to create a user library. When you choose this command, the Library Creation Wizard appears. The Wizard takes you through the steps of creating a search library or QC library.

A special command called **View Library** appears in the Analyze menu to allow you to view the contents of a library. For more information, find "library" in the OMNIC Help system Index and go to the "How to view a library in EZ OMNIC" topic.

Your First Experiment

⚠ Warning The *Spectrometer Safety Guide* that came with your system contains important safety information. This guide is available in several languages. Contact your local Thermo 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.

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.

Note If you have a dedicated system (such as a Liquid Analysis System) that normally uses a software package other than OMNIC or EZ OMNIC, skip this chapter.

In this first experiment you will...

- Select an experiment.
- Collect a background spectrum.
- Collect a sample spectrum.
- Save the sample spectrum in a file.

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

If a Smart Accessory is installed in the spectrometer, remove it before continuing. See the appropriate accessory tutorial available through Sampling Techniques in the Help menu of OMNIC for instructions. If you purchased the optional sample compartment cover, install it if it is not already installed. See “Installing the transmission sample compartment cover” in the “Servicing your spectrometer” book in Spectrometer Help Topics for instructions.

Things to check before you collect spectra

All the things you need to check before you collect spectra are listed below. 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.

⚠ Warning Liquid nitrogen is extremely cold and therefore potentially hazardous. Avoid contact with skin. Wear protective clothing eyewear and follow standard laboratory safety practices to prevent injury. Use an appropriate laboratory dewar to transport liquid nitrogen to the spectrometer.

- If you are using an MCT detector, fill the detector dewar (reservoir) with liquid nitrogen. Then allow the detector to cool for at least 20 minutes before collecting spectra. For instructions, view “Cooling a detector” in the “Using your spectrometer” book in Spectrometer Help Topics.

- Make sure the spectrometer, computer and printer are turned on and OMNIC is started. See “Turning on the system components” in the “Spectrometer Basics” chapter for details about turning on the power.

- Check the Power and Scan indicator lights near the rear-left corner on top of the spectrometer cover. The Power light should be on, and the Scan light should be on continuously or flashing. If this is not the case, follow the troubleshooting messages that appear or see the “Troubleshooting Hardware Problems” chapter of this manual for instructions.

- Check the purge filter (if present) and the humidity indicator. In Spectrometer Help Topics see “Checking and changing the purge gas filter” or “Checking the humidity indicator” in the “Maintaining your spectrometer” book.

Important The Avatar 370 CsI must be purged at all times to protect the CsI beamsplitter from being fogged by exposure to water vapor.

Selecting an experiment

The parameter settings for collecting spectra are stored in experiment files. You load the settings you wish to use when you select an experiment from the Experiment drop-down list box below the OMNIC menu bar (see the example below).

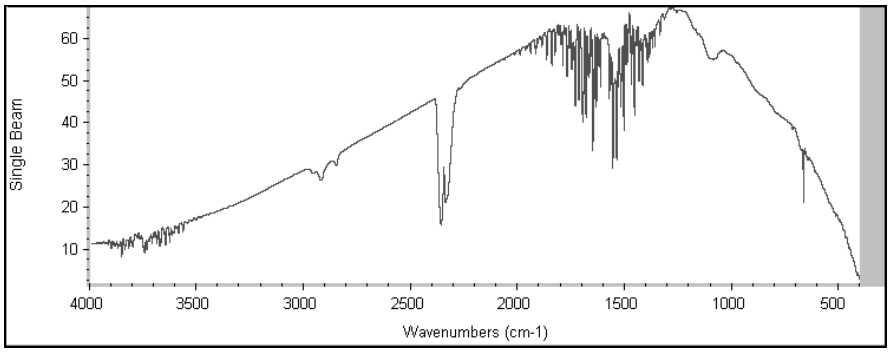
A number of experiments are included with OMNIC for performing a wide variety of data collections. You can open these experiments by choosing Open in the Experiment Setup dialog box. Experiment Setup is available in the toolbar and in the Collect menu. You can also use Experiment Setup to set up and save your own experiments, or to check or change the parameter settings after you select an experiment.

To learn more, view the “Collecting a Spectrum” tutorial, available through Learning OMNIC in the Help menu. If you need to change a source or detector, view “Replacing the source” or “Replacing the detector” in the “Servicing your spectrometer” book in Spectrometer Help Topics.

Collecting a background 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 mid-IR 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 usually necessary only if you are running quantitative experiments.)

Whenever you collect a background spectrum for a transmission experiment, make sure the sample compartment is empty (except for the transmission sample holder, if you are using it). You can initiate background data collection at any time by using the Collect Background button or Collect Background in the Collect menu.

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 about using Snap-In baseplates, choose Replacing Parts from the Help menu and then view "Changing the Snap-In baseplate" in "Installing optional hardware."

Collecting the sample spectrum

In the data collection procedure that follows, you will select an experiment and then collect a background spectrum and a polystyrene sample spectrum.

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

Follow these steps to collect the sample spectrum:

1. **Select an experiment.**

   To do this, first click the arrow button at the right end of the Experiment drop-down list box to display a list of available experiments. Here is an example:

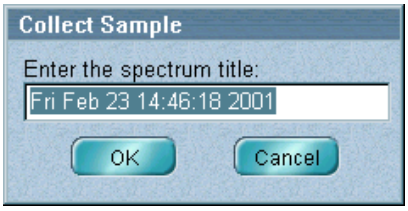
   The "Default - Transmission" experiment appears in the list. Select the experiment by clicking its name in the list.

   The parameters in the Experiment Setup dialog box are now set correctly for collecting a polystyrene sample spectrum. These parameters determine how OMNIC collects background and sample spectra. For example, in the experiment you selected, the Collect Background Before Every Sample option is selected. This option prompts you to collect a background before collecting the sample spectrum.

2. **Click the Collect Sample button in the toolbar.**

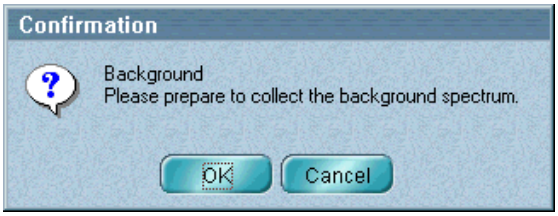
You can also choose Collect Sample from the Collect menu.

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

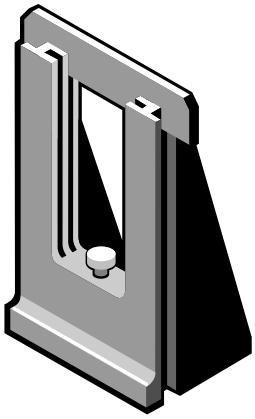


3. **Type a title in the text box and choose OK, or just choose OK to accept the default.**

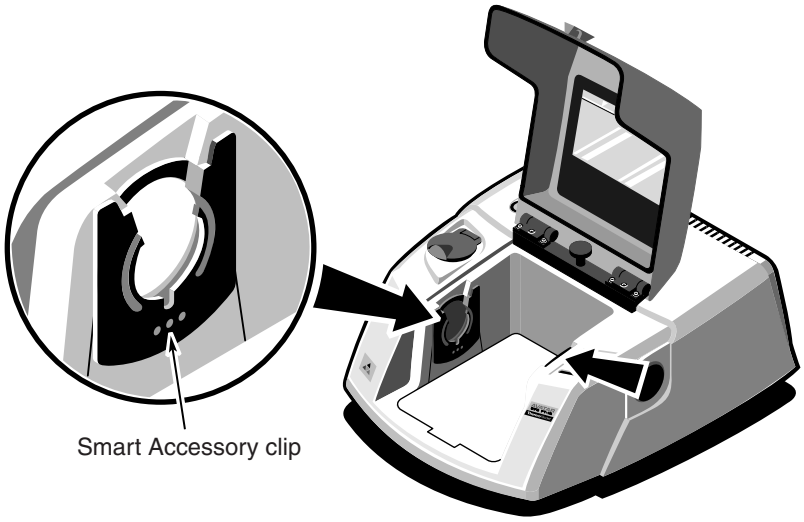
Since the experiment you are using specifies that a background be collected before every sample, a message appears asking you to prepare to collect a background spectrum:



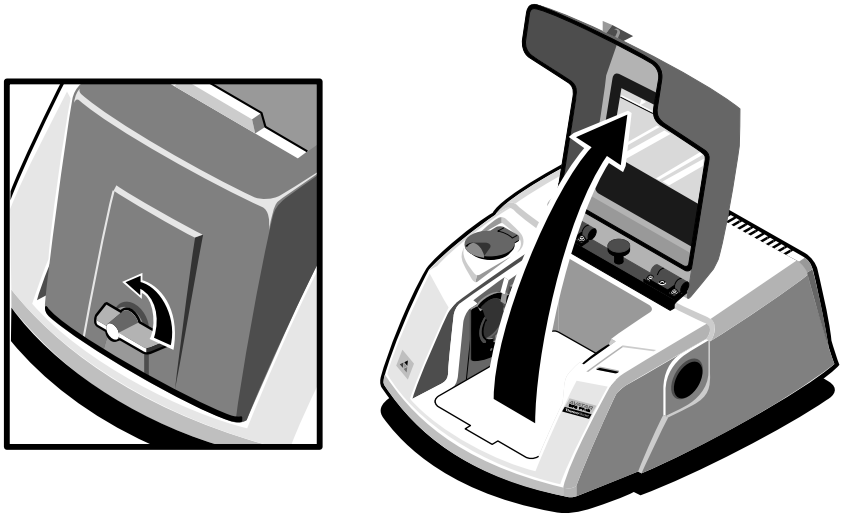
For a transmission experiment this means that you need to remove any accessories (other than a standard sample holder) and samples from the sample compartment, as explained in the next steps. A sample might be installed in the transmission sample holder...



...or in either of the Smart Accessory clips:



4. **If a sample is installed in the sample holder or Smart Accessory clips and the sample compartment cover is installed, open the cover by turning the latch and lifting the cover.**



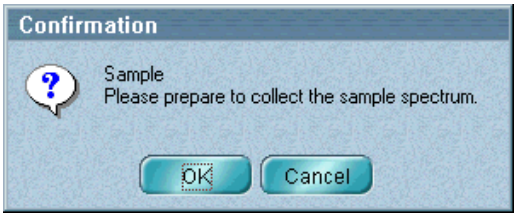
5. **If a sample is installed in the sample holder or Smart Accessory clips, pull the sample upward to remove it.**

6. **If you opened the sample compartment cover, close it after removing the sample.**

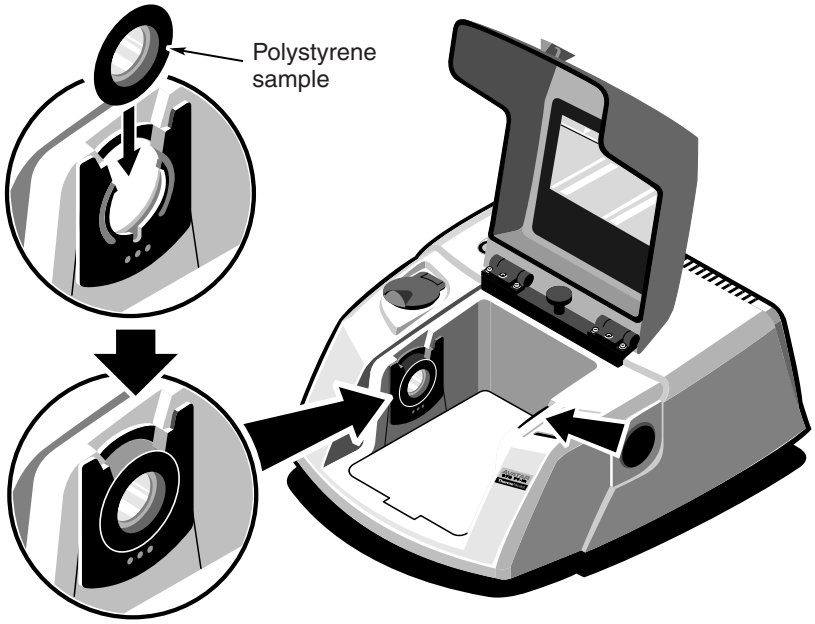
   If the spectrometer purged, allow 1 minute for the purge to reach equilibrium before going to the next step. If you find that carbon dioxide and water vapor interfere with spectra you collect in the future, wait 3 to 5 minutes.

7. **Choose OK to start background data collection.**

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



8. **Install the provided 0.0015-inch-thick polystyrene sample in either of the Smart Accessory clips.**

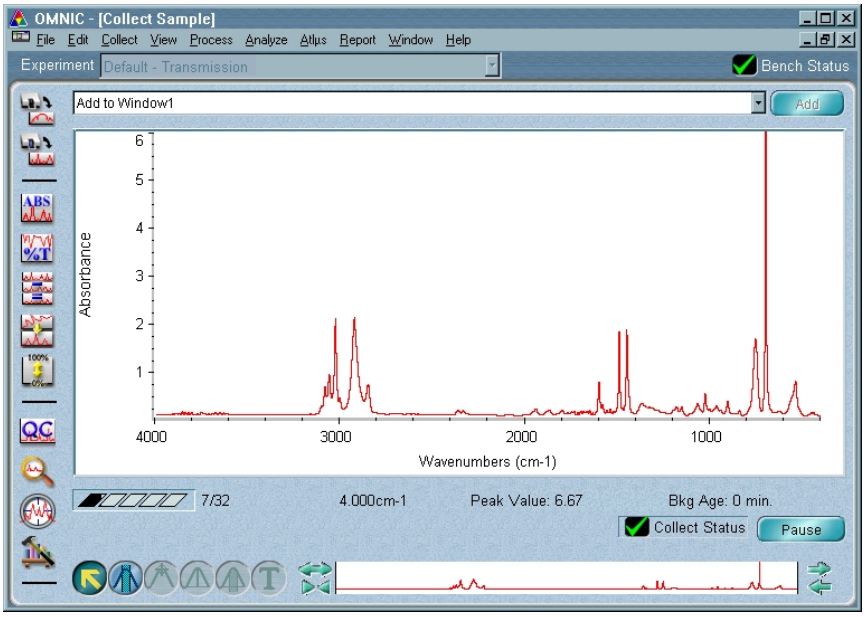


If the sample compartment cover is installed, open it, insert the sample and then close the cover. If your spectrometer purged, allow 1 minute for the purge to reach equilibrium before going to the next step.

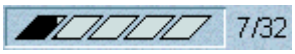
For more information about installing samples, view “Installing Samples” in the “Spectrometer Tour” tutorial available through Getting Started in the Help menu.

9. Choose OK to start collecting the sample data.

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

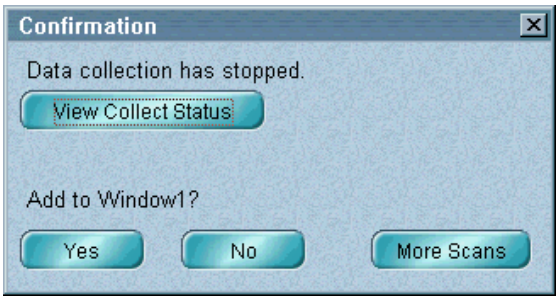


The progress of the collection is indicated by the gauge below the spectrum.



The number of scans collected so far and the total number of scans for the collection are displayed to the right of the gauge.

When data collection is finished, a message asks whether to add the spectrum to a spectral window:

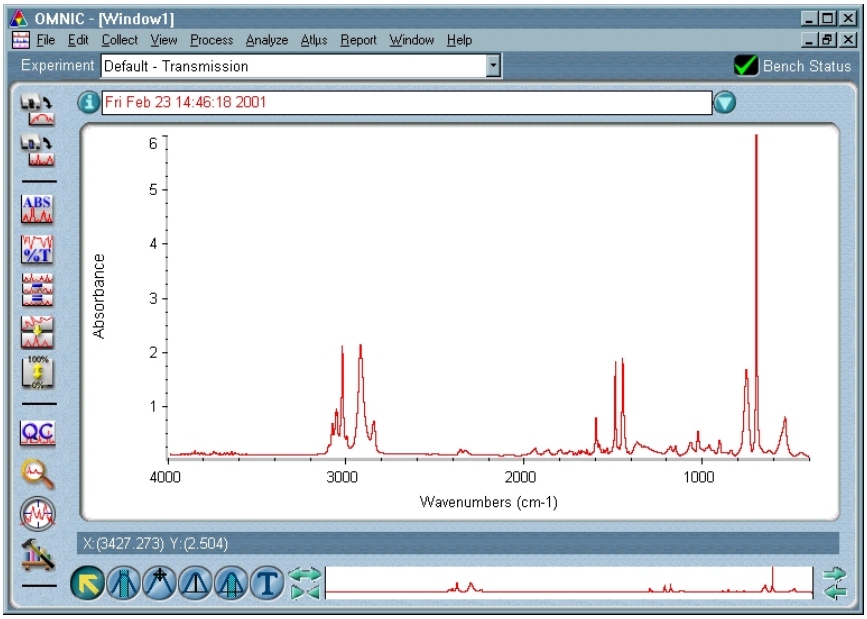


Note If Collect To A New Window is selected in the Collect options (available through Edit Options in the Edit menu), this message does not appear since the spectrum is placed into a new spectral window automatically.

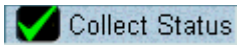
10. Choose Yes to add the sample spectrum to the spectral window.

Choosing No would end the procedure without saving the spectrum. Choosing More Scans would return you to the Collect Sample window, allowing you to collect more scans with the More button. Choosing View Collect Status would display information about the collection, including any problems that occurred (see the next section).

Here is an example of a sample spectrum displayed in the spectral window:



How do I know if my spectrum is good?



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

If you ever have a problem with data collection while one or more quality checks are turned on, the Collect Status indicator may change. If the indicator is a yellow circle, the spectrum has failed a spectral quality check (a measured value was not within the allowed range), but it is not serious enough to stop the collection. If the indicator is a red X, there is a problem with the quality of the spectrum. After correcting the problem, collect the spectrum again.

To view information about the collection, including a list of any problems that have occurred, click the Collect Status indicator during or after the collection. You can also click the View Collect Status button in the message that may appear when the collection is finished (see step 9 of the procedure in the preceding section). For each listed problem, an Explain button is provided to let you access troubleshooting information.

Saving the spectrum

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

Follow these steps to save the spectrum you just collected:

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

2. **Choose Save As from the File menu.**

   The Save As dialog box appears.

3. **Type a descriptive name (such as POLY.SPA) following the directory path in the File Name box.**

   Here is an example:

   C:\My Documents\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.

Using Other Basic Features of OMNIC

Once you know how to collect and save spectra, you can use other basic OMNIC features to...

- Convert a spectrum's units.
- Annotate a spectrum.
- Create and use spectral libraries.
- Create and view on-line laboratory notebooks.
- Control the optional validation wheel.

Converting a spectrum's units

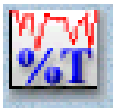
Typically the spectra you collect are in absorbance units or % transmittance units. Sometimes it is useful to convert a collected spectrum to other Y-axis units.

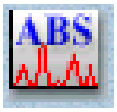
In this example you will convert the units of the spectrum you collected in the preceding chapter.

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

2. **If the spectrum is in absorbance, click the % Transmittance button on the toolbar. If the spectrum is in % transmittance, click the Absorbance button instead.**

You can also choose % Transmittance or Absorbance from the Process menu.





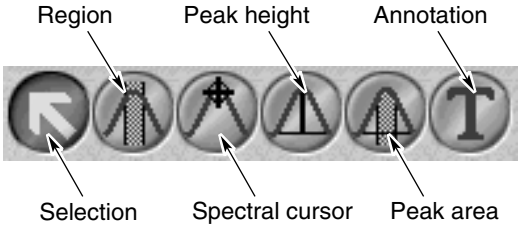
The spectrum's units are converted.

The toolbar buttons and the Process menu allow you to convert spectra to several other units as well. In OMNIC Help Topics find "converting spectrum" in the Index and go to the topic that deals with the units you are interested in.

Before going to the next section, convert the spectrum to absorbance so that it is ready for you to learn how to label a peak.

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.



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

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

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

1. **Select the annotation tool by clicking it.**

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

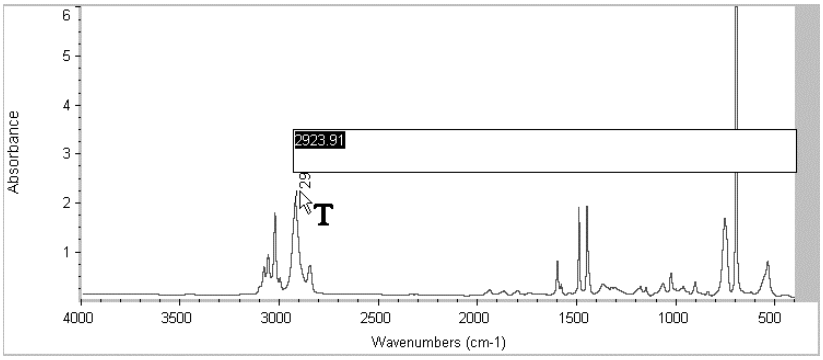
When the annotation tool is selected and you move the pointer into the spectral display, the pointer looks like this:

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

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

2. **Label a prominent peak by holding down the Shift key and clicking a little above the peak.**

   The label appears. Here is an example:



3. **Press Enter to accept the label text.**

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

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

In the next section, you will learn about using spectral libraries.

Using libraries

Spectra are often used to identify an unknown sample or to confirm a known sample's composition. To accomplish these tasks, the sample spectrum is compared with reference spectra contained in a library.

Libraries are collections of reference spectra. They may be a collection of commercially collected reference spectra, reference spectra you collected under controlled conditions, or simply a collection of spectra that you wish to store in an organized manner.

OMNIC lets you create these types of spectral libraries:

- Search libraries
- Quality control (QC) libraries
- Scrapbook libraries (not available in EZ OMNIC)

Searching

Search libraries are most often used to identify an unknown spectrum. If you are unsure of the composition of a sample, you can perform a "spectral search" using a search library.

We recommend using the "search expert" (if available in your version of OMNIC) to determine how to perform a spectral search and the kinds of search results to display. When a search is complete, the search expert displays a number of library spectra that best match the unknown spectrum, plus comments about the search results.

In OMNIC Help Topics find "library, searching" in the Index and go to the "Searching a spectral library" topic if you want more information about identifying sample spectra with search libraries.

Comparing

QC (Quality Control) libraries let you verify the composition of materials. These libraries are useful for quality control operations in which you know what a sample should contain and just need to verify and document the composition.

Spectra in QC libraries are stored in groups called “compound types.” This lets you maintain reference spectra that reflect variables in, or tolerances allowed for, your samples. The software compares your sample spectrum with the reference spectra in each compound type and reports the best match from each type.

QC comparisons are also useful for detecting minute differences in spectra. If you need to detect small changes (in the parts per million range) in your samples or identify samples that are spectroscopically very similar, you could create a QC library with as few as one reference spectrum in each compound type.

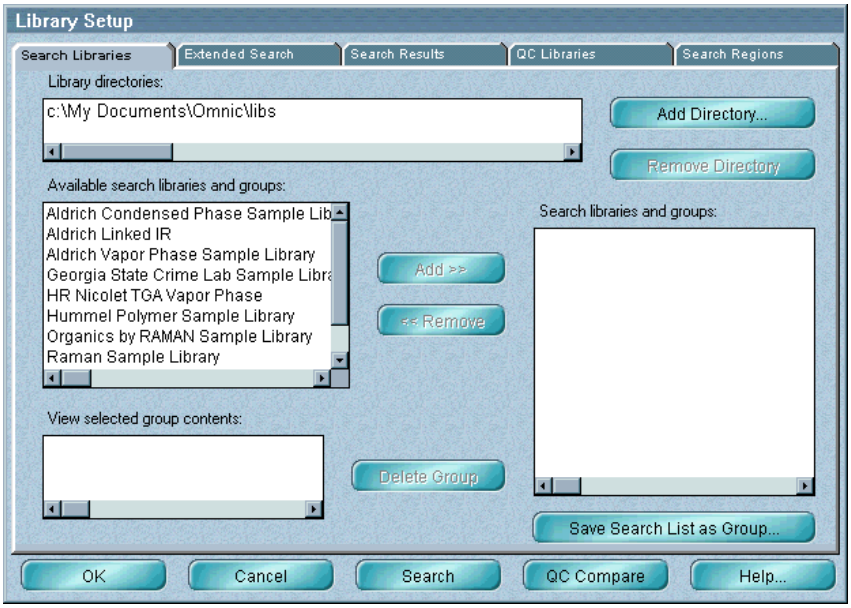
In OMNIC Help Topics find “QC comparison” in the Index and go to the “Performing a QC comparison” topic for more information about QC comparisons.

To try a QC comparison using your polystyrene spectrum, follow these steps:

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

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

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



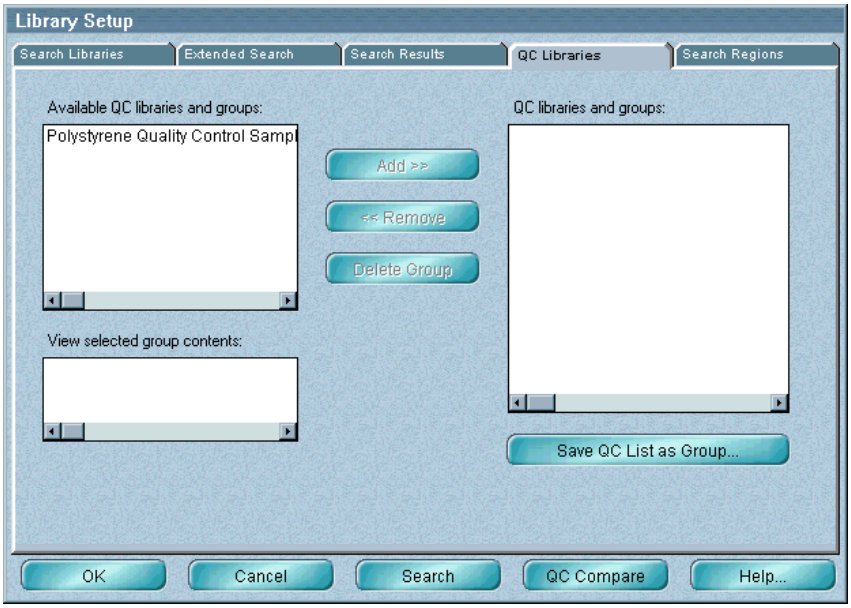
The Library Directories box lists the directories that are currently being used for spectral searches and QC comparisons. All the libraries in the listed directories are available for your QC comparison.

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

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

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

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



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

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

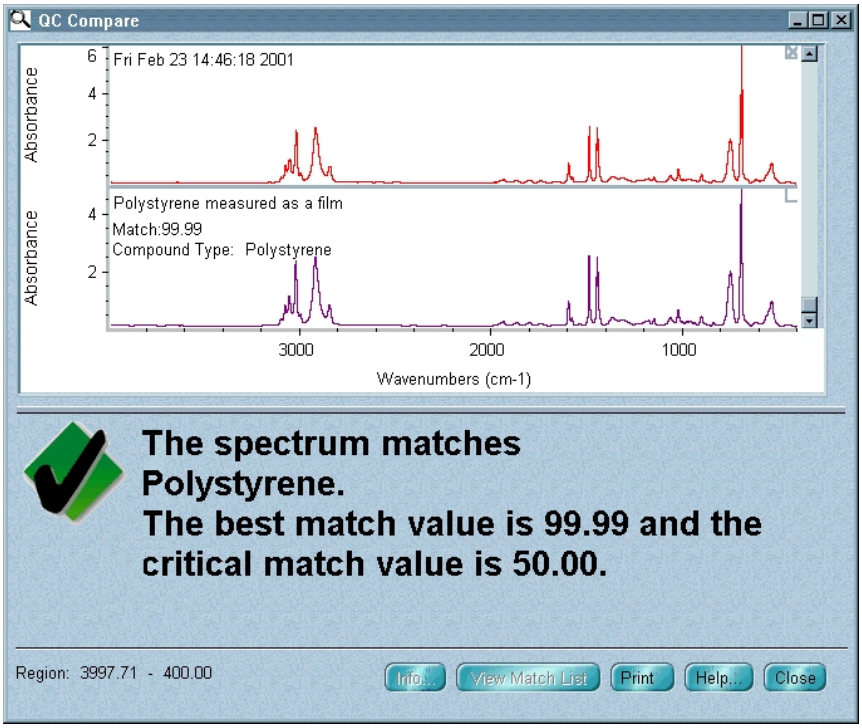
   To do this, click the appropriate library name in the Available QC Libraries And Groups box, and then click the Add button.

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

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

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

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



7. Close the QC Compare window by choosing Close.

Browsing

Scrapbook libraries are a convenient place to store and organize your spectra when you are using OMNIC. (Scrapbook libraries are not available in EZ OMNIC.) You can add any spectrum to a scrapbook library; the resolution and other parameters do not matter.

After you add spectra to a scrapbook library, you can find them by searching for text stored with the spectra. You cannot perform a spectral data search of a scrapbook library.

In OMNIC Help Topics find “library, searching for text in” in the Index and go to the “Searching a library for text” topic for more information.

OMNIC’s Library Manager (available in the Analyze menu) gives you the ability to view the spectra and related information contained in commercial and user libraries of spectra.

Note Library Manager is not available in EZ OMNIC. Use View Library in the Analyze menu instead to view library information.

Creating a user library

OMNIC’s Library Creation Wizard makes it easy to create your own spectral libraries. Creating your own library lets you customize the information in the library depending on your needs. You set the library parameters (including the resolution and spectral range) and specify which checks and corrections to perform. The wizard leads you step by step through the process.

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

If you are using EZ OMNIC, start the Library Creation Wizard by choosing Create Library from the Analyze menu.

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

Adding a spectrum to a user library

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

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

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

Creating and printing a report

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

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

1. **Choose Template from the Report menu.**

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

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

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

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

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

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

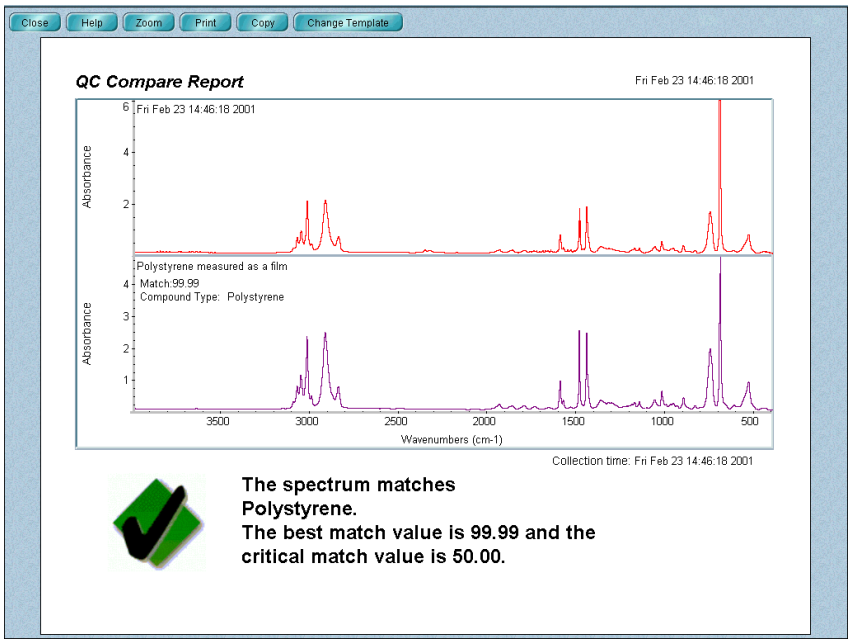
You can create your own report templates by using the Create button, or you can modify one of the existing templates whenever you want to design a new template. Save the template with a new name after you make your changes.

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

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

A preview of the report appears showing the report items filled in with information about your spectrum. Your report should look similar to this:

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



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

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

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

6. **Choose OK.**

   The report is printed on your system printer.

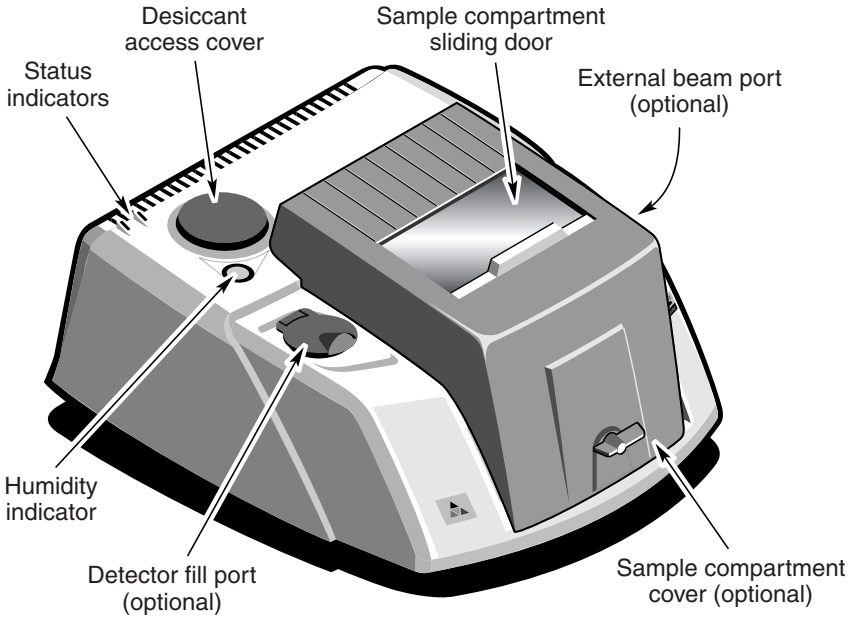
Spectrometer Basics

This chapter introduces the major components of your spectrometer, including the energy source, beamsplitter and detector. It also explains how to turn on the spectrometer power and describes what happens when the spectrometer starts up.

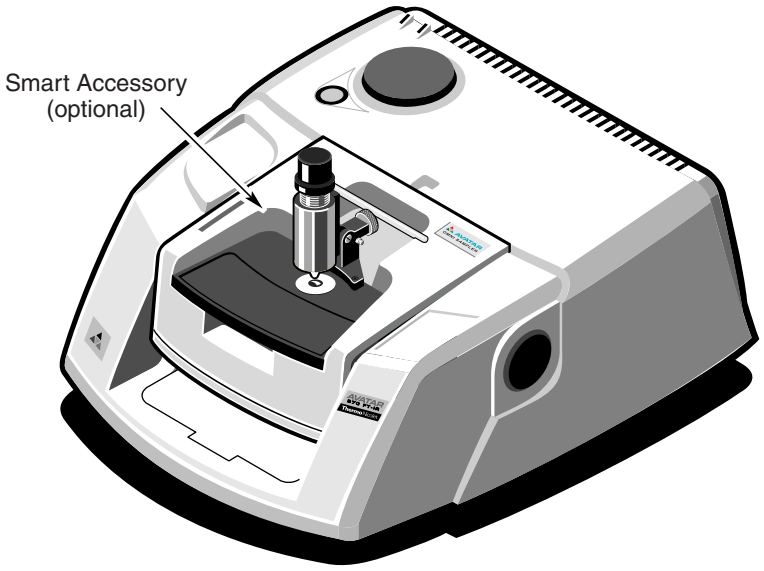
View the “Spectrometer Tour” tutorial available through Getting Started in the Help menu of OMNIC for complete descriptions of your spectrometer’s internal and external components.

Major spectrometer components

The following illustrations show Avatar spectrometers from the front, with different options installed.

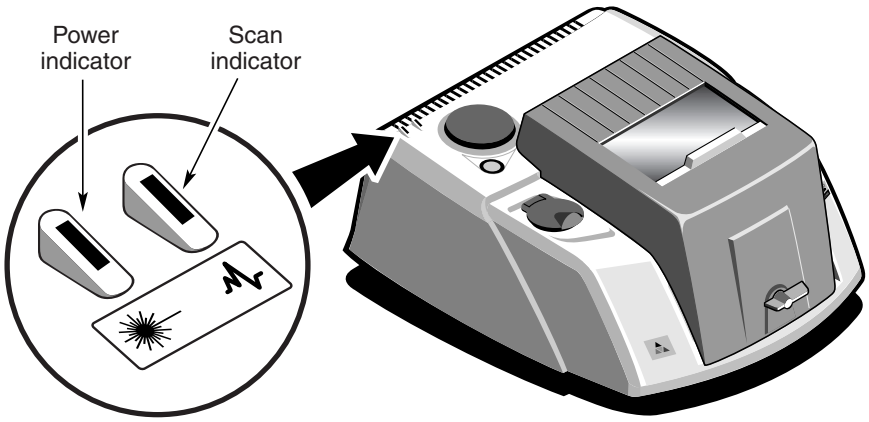


Avatar spectrometer with sample compartment cover



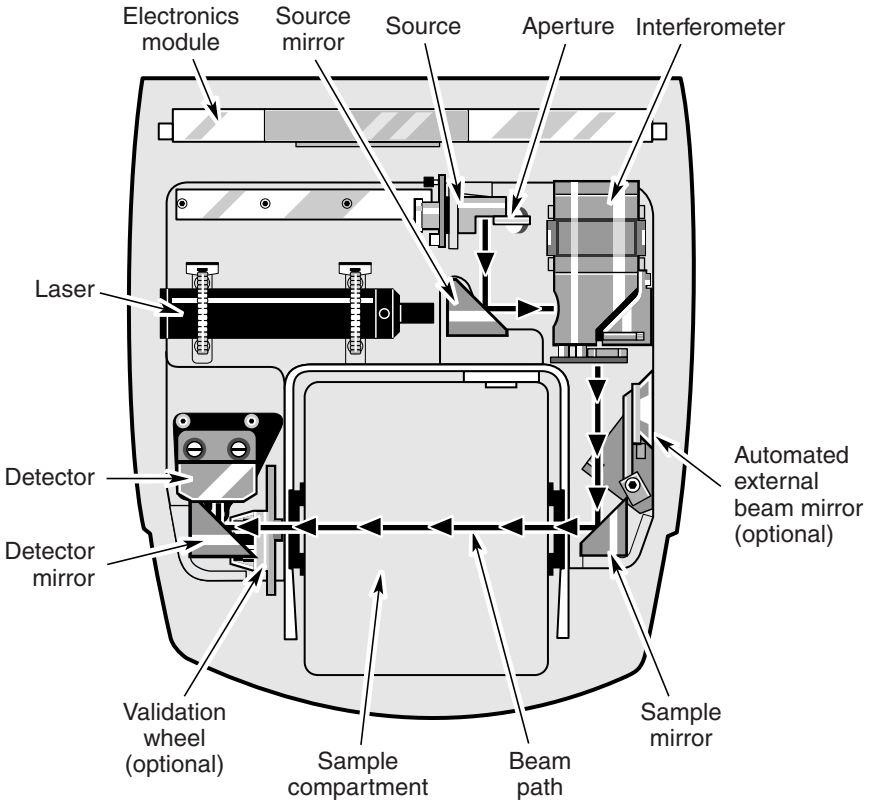
Avatar spectrometer with a Smart Accessory

The Power indicator is lit when the spectrometer power is on. The Scan indicator flashes when the spectrometer is scanning.



What's inside?

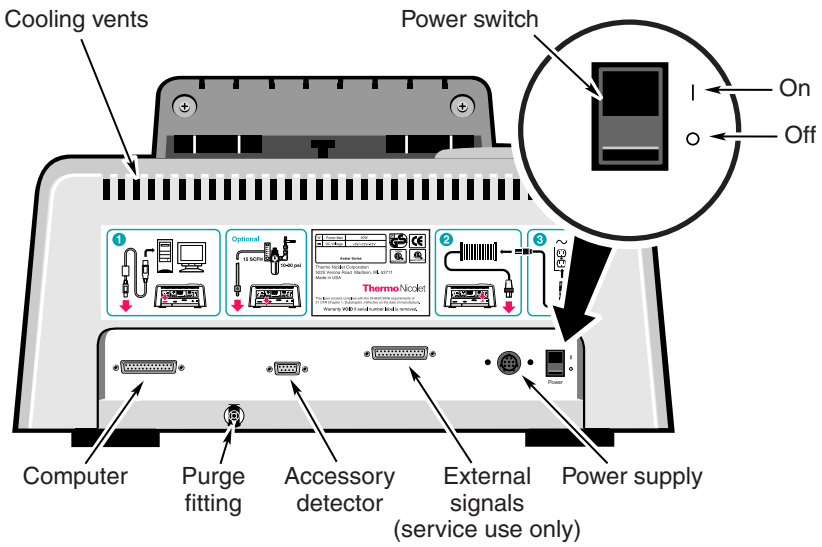
The illustration below shows a top view of the optical layout of an Avatar spectrometer with covers removed to reveal components.



View the "Inside the Spectrometer" unit of the "Spectrometer Tour" tutorial for complete descriptions of the internal components.

What is on the rear panel?

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



View the "The Back Panel" unit of the "Spectrometer Tour" tutorial for complete descriptions of the components on the rear panel.

Important Never block the cooling vents (see the preceding illustration). The electronics module inside the spectrometer could overheat if the vents are blocked.

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.**

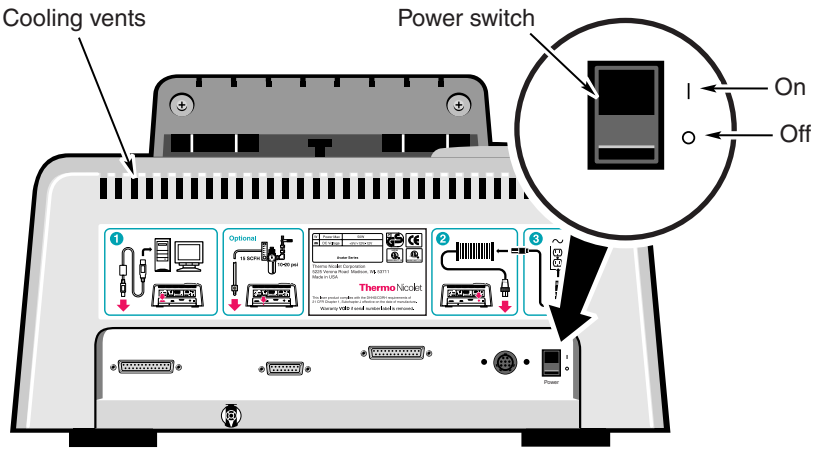
   This includes accessories such as an infrared microscope or a Liquid Analysis System.

2. **Turn on the computer and printer.**

   Follow the instructions that came with these components.

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

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



Important Never block the cooling vents (see the preceding illustration). The electronics module inside the spectrometer could overheat if the vents are blocked.

Note After you turn on the spectrometer, let it warm up for 15 minutes (one hour for best results) before collecting spectra.

When you turn on the spectrometer, the status indicators—Power and Scan—flash in various sequences as the system runs through its diagnostic routines. When the routines are finished, the Power indicator stays lit. You can start your spectroscopy software (OMNIC, EZ OMNIC or other Thermo Nicolet software) as soon as the diagnostic routines finish.

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

Note The system enters a “stand-by” 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 continuously. Any data collection activity will cause the interferometer to begin scanning. Exiting OMNIC also activates stand-by mode.

Note If the Power indicator flashes or does not light, or if the Scan indicator does not light, the Bench Status indicator in OMNIC will show a red X, and troubleshooting tips will appear on the screen. If you cannot resolve the problem, contact Thermo Nicolet at one of the numbers below. Outside the U.S.A. call your local sales or service representative. Telephone numbers for all Thermo Nicolet offices are provided with your system.

- Telephone (U.S.A.): 800-642-6538
- Fax: 608-273-6883
- World Wide Web: http://www.thermo.com/nicolet
- E-mail: techinfo@thermonicolet.com

More About Your Spectrometer

This chapter explains what you need to know before collecting spectra under various conditions. It includes information about hardware changes you can make to improve the precision and accuracy of your spectral data.

Sources, detectors and beamsplitters

The type of source, detector and beamsplitter in your spectrometer and the ability to change the source and detector depend on which Avatar model you have. Read the section that follows that pertains to your system.

If you need to replace or change the source or detector, view "Replacing the source" or "Replacing the detector" in the "Servicing your spectrometer" book in Spectrometer Help Topics.

Caution Even after the spectrometer is turned off, the external housing of the source remains 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.

For more information about using different sources, find "source" in the Index of OMNIC Help Topics and go to the "Specifying the source type" topic.

If you need to install an energy screen for the detector you are using, view "Energy screens" in the "Installing new hardware" book in Spectrometer Help Topics.

Avatar 330 source, detector and beamsplitter

The Avatar 330 has an Ever-Glo™ source, a DTGS-KBr detector and a permanently installed KBr beamsplitter. These components let you collect and analyze data in the 7,800 to 375 cm^{-1} spectral range. If your application requires data collection in other spectral ranges, contact your Thermo Nicolet representative for information about obtaining an optional Avatar 370 upgrade.

Avatar 370 source, detector and beamsplitter

The Avatar 370 is available in several source-beamsplitter-detector configurations. There are two main considerations when selecting a configuration: compatibility and spectral range. The following table lists the spectral ranges of compatible component combinations.

Beamsplitter	*Detector*	*Spectral Range (cm^{-1})*	*Source*
KBr	HP-DTGS-KBr	7,800 - 375	Ever-Glo
KBr	MCT-A*	7,400 - 600	Ever-Glo
CsI	DTGS-CsI	6,400 - 225	Ever-Glo

* This detector must be cooled with liquid nitrogen before use.

Improving the quality of your spectral data

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

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

The next sections explain how to optimize Avatar detectors to produce a more linear response and greater photometric accuracy, or to increase the signal-to-noise ratio.

How to improve the signal-to-noise ratio

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

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

If you have an Avatar 370, you can also switch to an energy screen that transmits more light or use no screen at all. However, the resulting spectrum might be distorted, and accuracy and stability could be reduced. (This is more likely to occur with an MCT detector than with a DTGS detector, which generally does not require the use of an energy screen.) See the next section for more about this.

View “Energy screens” in the “Installing new hardware” book in Spectrometer Help Topics for instructions on installing an energy screen.

How to improve linearity and photometric accuracy

Some detectors (such as MCT-A detectors) are highly sensitive and can become saturated or produce a distorted (nonlinear and photometrically inaccurate) signal if the light energy is not reduced before it reaches the detector element or if the detector gain is set too high.

Look at a single-beam spectrum in the low-end region around 600 to 375 cm^{-1}. You should see a straight line very near 0 intensity units. As a rule of thumb, the distance from 0 to the baseline should be less than 1% of the spectrum’s maximum intensity value. If the detector is saturated, you will see false energy in the low-end region. The baseline might be far above zero.

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

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 Thermo Nicolet Technical Support for assistance.

The distorted signal may cause problems with photometric accuracy. For good quantitative data, the sample and background interferograms should be about the same size. Scattering samples and very dense samples produce very small signals that, when compared with much larger background signals, can distort quantitative data.

Check the background and sample interferograms. If you see a substantial difference in their sizes, photometric accuracy could be a problem.

In some cases, system performance improves if you use a bandwidth-limiting filter or energy screen. 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. Energy screens help prevent detector saturation and signal distortion. See the next section for more information about using energy screens.

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.

View "Optical filters" or "Energy screens" in the "Installing new hardware" book in Spectrometer Help Topics for instructions.

Using energy screens

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

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

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

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

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

About the moving mirror velocity

Three moving mirror velocities are available for Avatar 370 and 370 CsI spectrometers: 0.4747, 0.6329 and 1.8988. (One velocity is available for the Avatar 330: 0.6329.) When you switch to a different detector, OMNIC automatically resets the default spectral range in the Experiment Setup dialog box. Be sure to check the range and set the velocity to a value that is appropriate.

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

For DTGS detectors, set Velocity to 0.63, or lower if you are analyzing a low-throughput sample. Higher velocities decrease the detector's sensitivity and increase the noise in your spectrum. (This is not a concern for MCT-A detectors; you can generally obtain good results using any available velocity setting.)

Accessories

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

Smart Accessories

In addition to traditional accessories, a variety of Smart Accessories are available for your spectrometer. The Avatar system identifies each Smart Accessory as soon as it is installed and set the software parameters for data collection. Also, a series of spectral quality checks are performed to ensure that the accessory is installed and operating correctly.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Other sampling accessories for different applications

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

Some accessories fit into the sample compartment and require that you remove the Snap-In baseplate before installing the accessory. For information on using Snap-In baseplates, view "Changing the Snap-In baseplate" in the "Using your spectrometer" book in Spectrometer Help Topics.

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

If you have an Avatar 330, an optional Avatar 370 upgrade is required for some accessories (as indicated below). See the next section for details about the upgrade.

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

Automated external beam mirror – If you have a microscope or other accessory with an external detector, this option is required. It directs the infrared beam out the port on the side of the spectrometer to the accessory whenever you select it. If you have an Avatar 330, an optional Avatar 370 upgrade is required.

Centaurμs™ and Continuμm™ infrared microscopes – Thermo Nicolet offers microscopes that attach directly to the right side of the spectrometer. Microscopes can be installed between the spectrometer and other accessory modules. The microscopes provide fast, nondestructive microanalysis with minimal sample preparation and alignment. If you have an Avatar 330, an optional Avatar 370 upgrade is required.

Gas cells – A variety of short- and long-pathlength gas cells are available. Cells include built-in transfer optics that fit into your spectrometer. 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.

Liquid Analysis System – This system lets you collect and process quantitative analysis data for liquid samples. It uses OMNIC Integra™ software, which contains methods for quantifying components in specific types of liquids. If you have an Avatar 330, an optional Avatar 370 upgrade is required.

Specular reflection accessories – Specular reflection provides a nondestructive method for measuring surface coatings without sample preparation. Specular reflection accessories can be used to analyze surface-treated metals, paints, semiconductors, and resin and polymer coatings.

Transmission E.S.P.™ accessory – Transmission is the oldest and most efficient sampling technique in FT-IR spectroscopy and can be used for sampling liquids, gases or solids. A variety of cells and sample holders are available for transmission analysis. All can be mounted in the spectrometer sample compartment. Thermo Nicolet's E.S.P. (Enhanced Synchronization Protocol) technology provides continuous communication between the accessory and OMNIC to ensure that the accessory is operating correctly.

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

System accessories

Some system accessories are installed by Thermo Nicolet. Call us if you are interested in ordering any of the following accessories.

Avatar 370 upgrade – If you have an Avatar 330 and you find that your applications require improved sensitivity, higher spectral resolution or external-beam capabilities, you can choose either a Customer Site or Factory Return upgrade package. These options give you access to...

- All OMNIC software products
- Enhanced performance
- High performance MCT-A detectors
- Other optional 370-only upgrades such as 0.5 cm^{-1} resolution or external beam experiments

Automated aperture – This option lets you perform high resolution (0.5 cm^{-1}) experiments. If you have an Avatar 330, an optional Avatar 370 upgrade is required.

Automated external beam mirror – This option lets you automatically direct the infrared beam out the port on the side of the spectrometer to an accessory such as a microscope or other accessory with its own detector. If you have an Avatar 330, an optional Avatar 370 upgrade is required.

Pure air generator – Thermo 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.

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

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

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

Purge kit – This kit includes all the hardware you need to regulate the pressure and flow of purge gas for your spectrometer. If you have difficulty controlling humidity in your laboratory or have a laboratory environment that is contaminated with solvents or other agents that can corrode spectrometer components, protect your spectrometer with a purge kit. Damage caused by humidity or corrosive agents is not covered by your Thermo Nicolet warranty.

RSVP™ (Remote Support and Verification Program) – This diagnostics 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.

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

Quick Answers to Your Questions About Using OMNIC

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

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

Collecting spectra

How do I set the software for collecting spectra?

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

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

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

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

How do I collect a spectrum?

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

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

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

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

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

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

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

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

What does gain do?

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

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

When should I save interferograms with my spectra?

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

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

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

What does the Collect Sample window show?

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

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

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

How do I know my spectra are meeting quality standards?

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

OMNIC offers four categories of spectral quality checks:

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

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

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

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

Converting spectra to other units

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

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

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

Use photoacoustic units for spectra collected using a photoacoustic accessory.

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

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

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

In the OMNIC Help Topics Index...

Find "absorbance" and go to "Converting spectra to absorbance."

Find "transmittance (%)" and go to "Converting spectra to % transmittance."

Find "Kubelka-Munk units" and go to "Kubelka-Munk units."

Find "photoacoustic units" and go to "Photoacoustic units" topic.

Find "reflectance (%)" and go to "% Reflectance units."

Find "log (1/R) units" and go to "Log (1/R) units."

Using spectral libraries

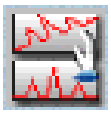
How do I search a spectral library?

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

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

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

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



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

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

- If the spectrum has totally absorbing bands, eliminate them by using Blank in the Process menu. Be careful not to blank regions that contain other important spectral information.

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

You can also use the region tool to select a region of the spectrum that does not include any totally absorbing bands or use the view finder to display the region before searching. (These methods avoid the loss of spectral information that results from blanking.)

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

- If you collected the spectrum using specular or diffuse reflection, use Kramers-Kronig (dispersion) correction (available through Other Corrections in the Process menu) to correct it for dispersion effects and then search it against a library of absorbance spectra.

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

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

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

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

In OMNIC Help Topics find “water” in the Index and go to “H2O and CO2 correction.”

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

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

How do I create a spectral library?

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

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

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

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

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

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

If you are using EZ OMNIC, use View Library in the Analyze menu.

In OMNIC Help Topics find “library” in the Index and go to “Working with libraries” or “Viewing a library or deleting a spectrum from a user library in EZ OMNIC.”

How can I find a compound in a commercial library?

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

If you are using EZ OMNIC, use View Library in the Analyze menu.

In OMNIC Help Topics find “library” in the Index and go to “Searching a library for text” or “Viewing a library or deleting a spectrum from a user library in EZ OMNIC.”

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

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

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

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

If you are using EZ OMNIC, you can add collected spectra to a user library with Add To Library in the Analyze menu.

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

What does the search expert do?

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

Opening, saving and deleting spectra

How do I open a stored spectrum?

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

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

How can I save my collected spectra automatically?

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

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

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

Where should I save my spectra?

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

For a permanent record of the spectrum and any other information you want to record, use a report notebook (not available in EZ OMNIC).

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

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

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

Note When you add a spectrum to user library whose resolution is lower, the spectrum is deresolved. For this reason it may be better in some cases to save your sample spectra as files on the hard disk and consider the copies of them added to a user library to be for searching purposes only.

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

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

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

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

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

How can I delete stored spectra?

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

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

Can I delete an entry from a report notebook?

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

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

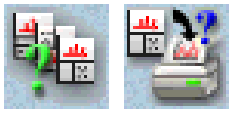
Printing

How can I specify a printer for printing information?

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

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

How can I create and print reports of my work?



Use the commands in the Report menu (not available in EZ OMNIC). First use Template to select, edit or create a template for the report. Then use Preview/Print Report to view the report as it will appear on paper. Click the Print button to print the report.

View Creating Reports (available through Learning OMNIC) to learn about OMNIC’s report features.

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

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

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

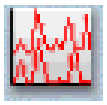
How can I preview spectra or other information before printing?

Use Preview/Print Report in the Report menu (not available in EZ OMNIC) to view a report as it would appear on paper. The report is displayed using the current report template; that is, the template you specified with Template or the one you are viewing and working with. If the report is displayed as you want it to appear on paper, you can print it by using the Print button.

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

Displaying spectra

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



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

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

How can I specify colors for displaying spectra?

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

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

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

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

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

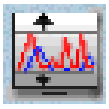
The parameters in the Display Setup dialog box affect the currently active spectral window only. The options in the Window options (in the Options dialog box, available through the Edit menu) affect all the new spectral windows that you create. After you create a new spectral window, you can change the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

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

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

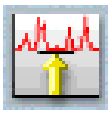
By using the appropriate command, you can display spectra so that they are easier to see or compare.

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



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

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



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

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

In the OMNIC Help Topics Index...

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

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

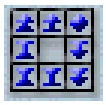
For information on Match Scale, find "spectra" and go to "Matching the Y scale of a spectrum."

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

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

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

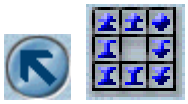
You can also click the top half of the Expand/Contract button at the left end of the view finder or drag the regions markers in the view finder to display a smaller spectral region.



In addition you can use Roll/Zoom Window in the View menu to expand an area.

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

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



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

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

How can I move a spectrum into another spectral window?

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

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

How can I move a stacked spectrum into another pane?

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

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

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

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

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

How can I find the height of a peak?

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

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

How can I find the area of a peak?

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

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

Should I correct the baseline of my spectrum?

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

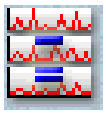
Correcting a baseline will give you better results when you search the spectrum against a library, subtract the spectrum from another spectrum, find peaks in the spectrum or quantify components in the spectrum.

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

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

Subtracting, adding, multiplying and dividing spectra

How can I subtract a spectrum from another spectrum?



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

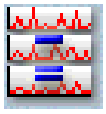
Select the spectrum from which you want to subtract spectral features; this is the sample spectrum. Then hold down the Control key and select the spectrum with the features you want to subtract from the sample spectrum; this is the reference spectrum.

Note Subtract is available only when two spectra are selected.

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

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

What should I use subtraction for?



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

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

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

What other mathematical operations can I perform on my spectra?

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

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

View Using Spectral Math (available through Learning OMNIC).

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

Customizing OMNIC

How can I customize my OMNIC software?

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

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

In the OMNIC Help Topics Index...

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

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

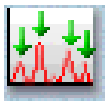
Find “toolbar” and go to “Customizing a toolbar.”

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

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

Other questions

How can I find and label peaks in spectra?



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

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

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

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

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

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

How can I select a spectral region for an operation?

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

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

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

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

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

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

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

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

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

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

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

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

- To see information about a particular feature in OMNIC, click the feature using the right mouse button. A brief description of the feature appears, and in most cases one or more buttons that you can click to display more detailed information. Click the Discussion button to display a complete discussion of the feature (or the dialog box or window that contains the feature). Click the How To button to display a step-by-step procedure for using the feature (or the dialog box or window that contains the feature).

- You can press the F1 function key at any time to see a discussion topic for the currently displayed or selected feature, dialog box or window.

- If a dialog box or window contains a Help button, click it to see information about the dialog box or window (or the command that displayed it).

- To see the Contents of the OMNIC Help system, choose OMNIC Help Topics from the Help menu.

Quick Answers to Your Questions About Using the Spectrometer

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

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

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

Spectrometer Help Topics...
"Energy screens" in "Installing new hardware"

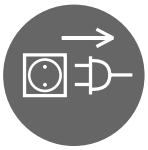
Do I need to use a bandwidth-limiting filter?

If you are using a highly sensitive detector such as an MCT-A 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. If you wish to use a bandwidth-limiting filter, you must supply your own.

Spectrometer Help Topics...
"Optical filters" in "Installing new hardware"

When do I need to open the spectrometer cover?

You need to remove the spectrometer cover to change sources or detectors or install a spectrometer component such as a laser or electronics module.



Warning: Do not operate the spectrometer with the main cover removed. 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 off the spectrometer power and unplug the power cord first. If you have an Avatar 370 CsI, protect the beamsplitter from the effects of water vapor by minimizing the time that the cover is removed.

Spectrometer Help Topics...
"Removing the main cover" in "Servicing your spectrometer"

When should I align the spectrometer?

Align the spectrometer in the following situations:

- The ambient temperature has changed by at least 5 Celsius degrees (about 9 Fahrenheit degrees).
- You are about to perform a spectrometer validation with Val-Q (or other software). This ensures that the validation is run with the best possible interferometer and electronics settings.
- The spectrometer power was turned off for more than a few minutes and has now been on for one hour.

Note We recommend that you leave the power on continuously, but if you do need to turn it off, allow the spectrometer to warm up for one hour and then align it before collecting spectra.

- The spectrometer has been on continuously for one week without being aligned. We recommended aligning your spectrometer once a week or, for optimum performance, once a day.
- You have just replaced the laser, source or detector.
- The detector signal intensity has dropped significantly from its usual level.
- You have just moved the spectrometer.

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

“Maintenance and Service” chapter...
“Aligning the spectrometer” in “Maintaining your spectrometer”

Does my detector need to be cooled with liquid nitrogen?

MCT detectors need to be cooled. These detectors have a dewar, a fairly large metal cylinder with a hole in the top. If during a work session you find that the detector signal intensity is decreasing, the dewar may need to be refilled with liquid nitrogen.

Spectrometer Help Topics...
“Cooling a detector” in “Using your spectrometer”

When should I change the desiccant?

When the humidity indicator on the spectrometer cover turns pink, change the desiccant packs. If the packs are printed with information about reactivation, you can bake them at the indicated temperature for the specified time and then store them in a desiccator until the next time you need to change the desiccant.

You should check the indicator every two months, more often if your laboratory is not air conditioned or the spectrometer is in a humid environment.

Spectrometer Help Topics...

"Checking the humidity indicator" or "Replacing the desiccant packs" in "Maintaining your spectrometer"

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

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

How can I diagnose problems with the spectrometer?

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

See the "Troubleshooting your spectrometer" and "Ordering parts" books in Spectrometer Help Topics for instructions on diagnosing spectrometer problems and ordering replacement parts.

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.

"Maintenance and Service" chapter

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

How do I replace parts in the spectrometer?

Spectrometer Help Topics...
“Servicing your spectrometer”

Maintenance and Service

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

⚠ Warning Perform *only* those procedures described in this chapter. If there are other problems, contact Thermo Nicolet at one of the numbers below. Outside the U.S.A. call your local sales or service representative. Telephone numbers for all Thermo Nicolet Customer Support offices are provided with your system.

- Telephone (U.S.A.): 800-642-6538 or 608-276-6373
- Fax: 608-273-6883
- World Wide Web: http://www.thermo.com/nicolet
- E-mail: techinfo@thermonicolet.com

See the “Troubleshooting your spectrometer,” “Ordering parts” and “Servicing your spectrometer” books in Spectrometer Help Topics for instructions on diagnosing spectrometer problems and ordering and installing replacement parts.

Running diagnostic tests on spectrometer components

If your system is not performing properly, you can use the Diagnostic tab of the Experiment Setup dialog box to check the performance of spectrometer components and determine the source of the problem.

Note OMNIC continuously monitors the operation of the spectrometer hardware and shows its status with the Bench Status indicator below the menu bar of the OMNIC window. See "Bench Status indicator" in the "Welcome!" chapter for more information.

Follow these steps to run the spectrometer diagnostic tests:

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

   Remove any samples and sampling accessories (except a transmission sample holder).

2. **Choose Experiment Setup from the Collect menu or the toolbar.**

   The Experiment Setup dialog box appears.

3. **Click the Diagnostic tab.**

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

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

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

5. **When you are finished viewing the information, choose OK.**

Maintaining your spectrometer

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

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

Aligning the spectrometer

To ensure optimum system performance (high signal intensity, low noise and good sensitivity), you should align the spectrometer at least once a week using the OMNIC software. See the answer to the question "When should I align my spectrometer" in the preceding chapter for more information.

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

Follow these steps to align the spectrometer:

1. **Remove any sample or accessory from the sample compartment (except a transmission sample holder).**

   The beam path must be clear during alignment. If your spectrometer is purged, open the sample compartment as briefly as possible to maintain a constant purge.

2. **Choose Experiment Setup from the Collect menu or the toolbar.**

   The Experiment Setup dialog box appears.

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

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

Important Do not use Autogain.

5. **Click the Align button on the Diagnostic tab.**

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

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

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. (This practice does not include Smart Accessories, which do not require alignment.) First align the spectrometer without the accessory installed, as described in the preceding section. 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 (attenuated total reflection) 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 in the live display on the Bench tab. 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 on the Bench tab before adjusting the accessory. The tone reaches its highest pitch when the signal is maximized.

Checking spectrometer performance

You can use the performance test to track long-term spectrometer performance. Run the test 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 inside 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 perform the performance test:

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

   Remove any samples and sampling accessories (except a transmission sample holder).

2. **Exit OMNIC.**

   This ensures that the Bench Diagnostics software will run correctly.

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

   To do this, click the Start button on the Windows taskbar, point to Programs (All Programs in Windows XP), point to the Thermo Nicolet folder and then choose Bench Diagnostics.

See “Performing advanced diagnostic tests” in the “Troubleshooting Hardware Problems” chapter for more information on running the Bench Diagnostics software.

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

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

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

Checking the purge

If your spectrometer is equipped with an optional purge kit, make sure the pressure regulator is set between 0.7 and 1.4 bar (70 and 140 kPa, or 10 and 20 pounds per square inch) and the flowmeter is set to 15 standard cubic feet per hour (about 0.4 m^3/hr).

Note Excessive purge flow rates can introduce noise into your spectra. Do not exceed 15 scfh.

Important The Avatar 370 CsI must be purged at all times to protect the CsI beamsplitter from being fogged by exposure to water vapor.

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

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

In Spectrometer Help Topics view "Setting the purge gas controls" in the "Using your spectrometer" book and "Checking and changing the purge gas filter" in the "Maintaining your spectrometer" book for information about how to install the purge equipment, set the controls for the first time, and inspect and clean the purge filter.

Servicing your spectrometer

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

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

If the source, laser module, electronics module or power supply must be replaced, refer to the replacement parts list made available when you choose Spectrometer Help Topics from the Help menu. Call 800-642-6538 or 608-276-6373 to order the replacement assembly. If you are outside the U.S.A., contact your local Thermo Nicolet office. Telephone numbers for all Thermo Nicolet Customer Support offices are provided with your system.

Troubleshooting Software Problems

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

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

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

Problem	Possible Cause	Solution
You cannot add a spectrum to a user library.	The resolution of the spectrum is lower (higher numerical value) than that of the library. The spectrum is from a commercial library.	Collect the spectrum at the same resolution as the library (first set Resolution on the Bench tab of the Experiment Setup dialog box) and then add it to the library. Only spectra you collect can be added to a user library. Commercial libraries cannot be altered and the spectra contained in them cannot be copied to other libraries.
An experiment provided with OMNIC does not produce good results.	The parameter settings in the experiment file have been changed so that the experiment is no longer useful.	Restore the experiment to its default settings: First open the experiment using Experiment Setup and save it using a new filename if you do not want to overwrite it. Then open the experiment in the FACTORY directory whose filename is same as the original experiment and save it in the OMNIC\PARAM directory.
The desired experiment does not appear in the Experiment drop-down list box.	The experiment was installed with the software but has not yet been opened.	If the experiment was designed for a Smart Accessory, install the accessory; the experiment will be opened automatically and will appear in the Experiment drop-down list box. If the experiment was not designed for a Smart Accessory, open it using Experiment Setup; it will be added to the list.
Libraries created with previous version of OMNIC are not listed in the Library Setup dialog box.	The libraries are not in one of directories listed in the dialog box (typically LIBS within the OMNIC directory).	Use the Add Directory button on the Search Libraries tab to add the directory.

Troubleshooting Hardware Problems

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

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

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

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

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

Problem	Possible Cause	Solution
There is frost on the outside of the detector.	The insulating vacuum chamber of the dewar has begun to leak.	If you suspect your detector has a vacuum leak, view “Maintaining detector dewars” in the “Maintaining your spectrometer” book in Spectrometer Help Topics.
A message says that data cannot be collected.	The spectrometer is turned off.	Turn on the spectrometer and wait until the start-up diagnostics finish before restarting OMNIC.
	The data cable is loose, disconnected or damaged.	Shut down the computer and turn off the spectrometer. Check the data cable. If it is damaged, replace it. If the cable is loose or disconnected, reconnect it. Turn on the spectrometer and wait until the spectrometer start-up diagnostics finish. Then turn on the computer and restart OMNIC.
	The parallel port in the computer is not configured correctly.	Make sure that the computer parallel port is in ECP mode. Use the instructions that came with your computer.
	A component has failed.	Contact Thermo Nicolet for service.

Problem	Possible Cause	Solution
Data is not displayed during collection.	The data cable between the spectrometer and computer is not properly connected.	Turn the spectrometer power off and check the data cable connections.
	The spectrometer is out of alignment.	Align the spectrometer using the Align button on the Diagnostic tab of the Experiment Setup dialog box.
	The laser is not functioning.	Click the laser indicator on the Diagnostic tab of the Experiment Setup dialog box to check the laser operation. Call Thermo Nicolet to order a replacement laser if necessary. See the "Ordering parts" and "Servicing your spectrometer" books in Spectrometer Help Topics to find part number and ordering and installation instructions.
	The spectrometer is overheated. (You can check whether the temperature of the electronics board is within the acceptable range by clicking the electronics indicator on the Diagnostics tab of the Experiment Setup dialog box.)	Make sure the cooling vents on the back of the spectrometer are not blocked and nothing is stacked on top of the spectrometer. Maintain at least 30 cm (12 in) of clearance behind the spectrometer and 64 cm (25 in) of clearance above the table. Make sure the ambient temperature is between 16° and 27°C (60° and 80°F).

Problem	Possible Cause	Solution
The status indicators on the spectrometer cover do not light when the spectrometer is turned on.	The power supply connection on the back of the spectrometer is loose.	Turn off the spectrometer and check the connections between the spectrometer and the power supply. Make sure the lock ring is tightened finger-tight.
	The spectrometer is not plugged in.	Make sure the power cord is securely connected to the power supply and a working outlet or power strip.
	The power cord is not properly rated for your electrical service.	Make sure the power cord is appropriate for your AC power source. In Spectrometer Help Topics see “Miscellaneous parts” in the “Ordering parts” book for power cord descriptions and part number information.
	The ground prong on the power cord has been removed or is defective.	Replace the power cord. In Spectrometer Help Topics see “Miscellaneous parts” in the “Ordering parts” book for power cord descriptions and part number information.
	The power cable or power supply is defective.	Look through the holes near the power switch on the rear panel to check the power LEDs. All three green LEDs light when the power supply is working properly. If any are not lit, call Thermo Nicolet to order a cable or power supply.

Problem	Possible Cause	Solution
The signal intensity is low. (Also, the Scan indicator may flash intermittently and the spectrometer alignment may fail.)	The source is glowing unevenly.	Check to see if the source element is glowing evenly. Order a replacement source if needed.
	The beam path is obstructed.	Remove the obstruction.
	The sample compartment KBr windows are fogged.	Call Thermo Nicolet to have the windows replaced.
	The beamsplitter is fogged.	Check the laser signals by clicking the laser indicator on the Diagnostic tab of the Experiment Setup dialog box. If you suspect the beamsplitter is fogged, call Thermo Nicolet for service.
	The spectrometer is out of alignment.	Align the spectrometer using the Align button on the Diagnostic tab of the Experiment Setup dialog box.
	A sampling accessory is not installed properly.	Make sure the accessory is installed according to the instructions that came with it.
	A detector that was just installed is not seated properly.	Make sure the hole and slot in the detector plate fit over the pins on the spectrometer baseplate. See "Replacing the detector" in the "Servicing your spectrometer" book in Spectrometer Help Topics.

Problem	Possible Cause	Solution
The system scans normally but gives very low signal intensity.	The spectrometer is out of alignment.	Align the spectrometer using the Align button on the Diagnostic tab of the Experiment Setup dialog box.
	The moving mirror velocity is set too high.	Set Velocity on the Bench tab of the Experiment Setup dialog box to a lower velocity.
	There is no interferogram.	If the Source status indicator is off, click the source indicator on the Diagnostic tab of 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 of the Experiment Setup dialog box; if the interferogram is not present, check the beam path and detector.
	The beam path is obstructed.	Remove the obstruction.
	The optional automated aperture is set incorrectly.	Check the Aperture parameter on the Bench tab of the Experiment Setup dialog box. For an MCT-A detector, set Aperture to 10. For a DTGS detector, set Aperture to 100.
	Continued on next page...	

Problem	Possible Cause	Solution
	...continued	
	The spectrometer is overheated. (You can check whether the temperature of the electronics board is within the acceptable range by clicking the electronics indicator on the Diagnostics tab of the Experiment Setup dialog box.)	Make sure the cooling vents on the back of the spectrometer are not blocked and nothing is stacked on top of the spectrometer. Maintain at least 30 cm (12 in) of clearance behind the spectrometer and 64 cm (25 in) of clearance above the table. Make sure the ambient temperature is between 16° and 27°C (60° and 80°F).
	A sampling accessory is not installed properly or is not aligned.	Make sure the accessory is installed correctly and, if necessary, align it. See the instructions that came with the accessory.
An error message appears when you try to scan.	The light source is not working.	Check the source indicator on the Diagnostic tab of the Experiment Setup dialog box. If necessary, replace the source.
	An MCT detector is not cooled.	Check and cool the detector.
	The interferogram peak is not located at 1024 ± 16 data points on the Bench tab of the Experiment Setup dialog box.	Align the spectrometer. If the interferogram is still not located correctly, call Thermo Nicolet for service.
	The beam path is obstructed.	Remove the obstruction.
	The data cable between the spectrometer and the computer is not properly connected.	Turn off the spectrometer power and check the data cable connections.

Problem	Possible Cause	Solution
The Scan status indicator does not flash (the system is not scanning). (Note: After 1 hour without data collection activity, the interferometer stops scanning and the Scan light stays on. This is normal. Any data collection activity will cause the interferometer to begin scanning.)	The spectrometer is turned off.	Turn on the spectrometer power.
	The spectroscopy software has not been started.	Start OMNIC (or other software you are using).
	The spectrometer is out of alignment.	Align the spectrometer using the Align button on the Diagnostic tab of the Experiment Setup dialog box.
	The electronics module needs to be reset.	Turn off the power to the computer and the spectrometer. Leave the power off for 15 seconds. Turn on the spectrometer and wait until the start-up diagnostics finish. Then turn on the computer and restart OMNIC.
	The laser is flickering.	Click the laser indicator on the Diagnostic tab of the Experiment Setup dialog box to check the laser operation. Call Thermo Nicolet for assistance.
	The laser is off.	Turn off the spectrometer power, unplug the power cord, remove the spectrometer cover and make sure the laser cable is seated properly. See "Replacing the laser" in the "Servicing your spectrometer" book in Spectrometer Help Topics for instructions. **Warning:** Do not open the spectrometer cover without first turning off the power and unplugging the power cord.
	Continued on next page...	

Problem	Possible Cause	Solution
	...continued	
	The laser or electronics module is defective.	Check the laser indicator on the Diagnostic tab of the Experiment Setup dialog box. If there is a red slash through the laser indicator, click the indicator to view information about the laser operation. If the laser frequency is outside the specified range, call Thermo Nicolet to have the electronics module replaced. If the laser voltage or current is outside the specified range, replace the laser. View "Replacing the laser" in the "Servicing your spectrometer" book in Spectrometer Help Topics for instructions.
	The spectrometer is overheated. (You can check whether the temperature of the electronics board is within the acceptable range by clicking the electronics indicator on the Diagnostics tab of the Experiment Setup dialog box.)	Make sure the cooling vents on the back of the spectrometer are not blocked and nothing is stacked on top of the spectrometer. Maintain at least 30 cm (12 in) of clearance behind and 45 cm (18 in) of clearance above the spectrometer. Make sure the ambient temperature is between 16° and 27°C (60° and 80°F).
	A component has failed.	Call Thermo Nicolet for service.

Problem	Possible Cause	Solution
The baseline is not stable.	The purge flow rate is too high.	Lower the flow rate until the baseline is stable.
	The spectrometer is out of alignment.	Align the spectrometer using the Align button on the Diagnostic tab of the Experiment Setup dialog box.
	The center laser detector is misaligned.	Use the Bench Diagnostics software 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 of the Experiment Setup dialog box. If the levels remain out of tolerance, call Thermo Nicolet for service.
	The ambient conditions are outside the allowed ranges.	Make sure the conditions meet the requirements given in the "Environmental Considerations" chapter of *Preparing Your Site*.
	The desiccant cannot absorb any more water vapor.	Check the humidity indicator and replace the desiccant and indicator if needed.
	The spectrometer cover was recently opened.	Allow the spectrometer to purge for 3 to 5 minutes after the cover is closed.
You encounter problems when selecting an external detector in a microscope.	The detector cable is loose at the accessory connector (on the rear of spectrometer or on the back wall of the sample compartment).	Check and tighten the cables.

Performing advanced diagnostic tests

You can use the Bench Diagnostics program to perform diagnostic tests on the main components of the spectrometer. You should run these tests if you have problems with your spectrometer to determine the cause. The diagnostics provide information about the status of the component as well as troubleshooting information, replacement procedures and information about ordering replacement parts.

Use the diagnostics software to:

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

Follow these steps to run the diagnostics:

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

   Remove any samples and sampling accessories (except a transmission sample holder).

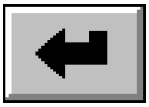
2. **Start the Bench Diagnostics software.**

   To do this, choose Advanced Diagnostics from the Collect menu. You can also close OMNIC (or EZ OMNIC), click the Start button in Windows, point to Programs (All Programs in Windows XP), point to the Thermo Nicolet folder and then choose Bench Diagnostics. This gives you access to advanced features of the software, including the performance test, that are not available if you run the diagnostics from OMNIC.

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

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

   Click this button to return to the main Diagnostics window:



   To exit the Bench Diagnostics software, click the Close button at the far right end of the title bar.

Troubleshooting Applications Problems

If you have turned on OMNIC's spectral quality checks feature, the software automatically checks the status of collected interferograms, and background and sample spectra. When OMNIC performs a check and detects a problem with data collection or spectra, the Collect Status indicator is displayed as a yellow circle or a red X. You can click the indicator (or click the View Collect Status button at the end of data collection) to see a summary of data collection problems encountered during the collection and other information about the collection.

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

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

Problem	**Possible Cause**	**Solution**
A spectrum contains fringes or channeling.	The sample has parallel, highly reflective sides that cause the infrared beam to bounce within the sample when it is placed perpendicular to the beam.	Create a new film using a matte press. Try roughening the film surface slightly with silicon carbide paper or other suitable abrasive. Rotate the sample so that the infrared beam passes through sample at Brewster's angle. (Do not use this method if you are performing a quantitative analysis of sample.)

Problem	Possible Cause	Solution
A spectrum contains totally absorbing peaks.	The sample in a transmission experiment is too thick.	Use a thinner sample.
A spectrum contains carbon dioxide peaks that interfere with your data.	The background spectrum is too old.	Collect a new background spectrum to use for ratioing your sample spectra.
	The spectrometer is not adequately purged.	Make sure you are using the correct purge gas and that purge flow rate is adequate. Allow the system 3 to 5 minutes to reestablish purge before collecting the spectrum.
	The spectrometer is not purged.	Install an appropriate purge gas source and optional purge kit. Contact Thermo Nicolet for details.
	The spectrometer is purged but the air dryer does not remove carbon dioxide.	Replace the air dryer with one that removes carbon dioxide, or use nitrogen to purge the spectrometer. Contact Thermo Nicolet for more information.
A spectrum contains water peaks that interfere with your data.	The desiccant cannot absorb any more water vapor.	Check the humidity indicator and replace the desiccant and indicator if needed.
	The spectrometer is not adequately purged.	Make sure you are using the correct purge gas and that purge flow rate is adequate. Allow the system 3 to 5 minutes to reestablish purge before collecting the spectrum.
	The spectrometer is not purged.	Install an appropriate purge gas source and optional purge kit. Contact Thermo Nicolet for details.

Problem	Possible Cause	Solution
A spectrum contains no peaks.	No sample is in the infrared beam path.	Check the sample compartment or accessory to make sure the sample is properly positioned in the beam path.
	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. For more information, view the appropriate tutorial available through Sampling Techniques in the Help menu.
	An infrared microscope is in its viewing mode.	Put the microscope in infrared mode and collect the spectrum again.
	A sample film in an 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.
	The resolution is set too low.	Set Resolution on the Collect tab of the Experiment Setup dialog box to a value that lets you see small peaks. (Use a lower numerical setting to achieve higher resolution.)
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.

Problem	Possible Cause	Solution
The baseline of the spectrum is not flat.	The 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 of 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 the correct purge gas is being used and that the flow rate is correct.

Problem	Possible Cause	Solution
A spectrum is too noisy.	There were too few scans.	Increase the number of scans on the Collect tab of the Experiment Setup dialog box.
	The resolution was too high.	Reduce the resolution (use a higher numerical setting) on the Collect tab of the Experiment Setup dialog box.
	The purge gas flow rate or pressure is too high.	Check the pressure regulator; it should be set between 0.7 and 1.4 bar (70 and 140 kPa, or 10 and 20 psig). Check the flowmeter; it should read 15 scfh (about 0.4 m^3/hr). Adjust the flow rate if necessary.
	The detector is saturated.	Add a bandwidth-limiting filter or an energy screen to reduce the signal strength.
	The moving mirror velocity is set too high for the detector.	Set Velocity on the Bench tab of the Experiment Setup dialog box to a lower value.
	The sample in an ATR experiment is not in good contact with the ATR crystal.	Reapply the sample to obtain more consistent contact between the sample and the ATR crystal.

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