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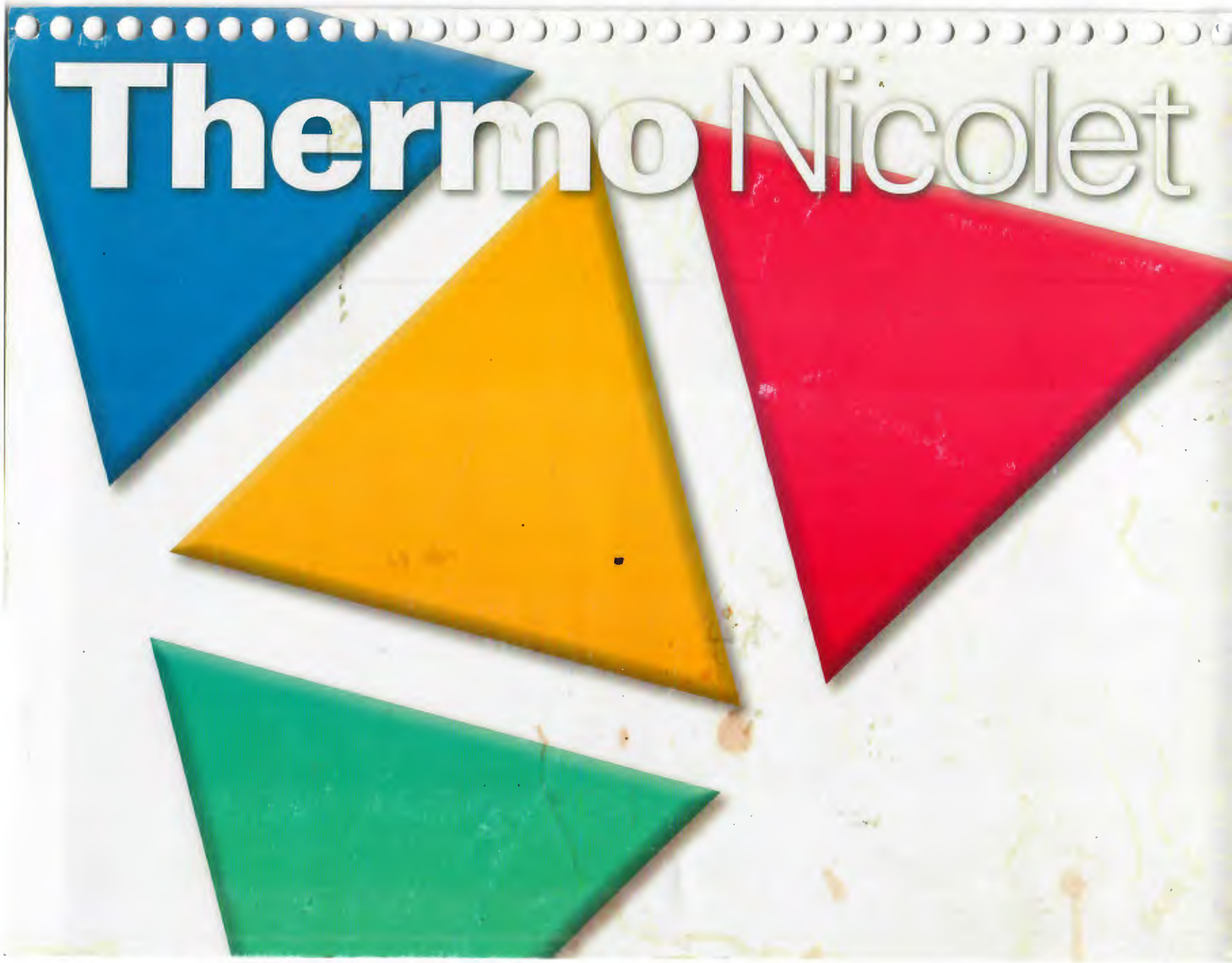
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AVATAR

360 System User's Guide

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

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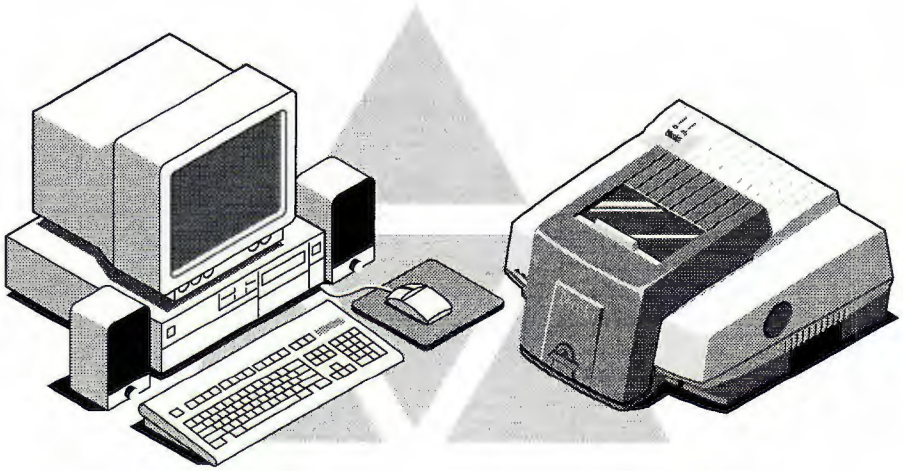
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Welcome to Avatar 360!

Congratulations on your purchase of an Avatar™ 360 E.S.P.™ spectrometer! The spectrometer lets you collect spectra in either the mid-IR or near-IR spectral ranges. The E.S.P. system integrates advanced hardware features with the power and flexibility of Nicolet's OMNIC® software‡.



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

---

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

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If you have questions or concerns

If you have any questions or concerns about your Avatar spectrometer, contact Nicolet Customer Support at one of the numbers below. Outside the U.S.A. call your local sales or service representative. Telephone numbers for all Nicolet Customer Support offices are provided with your system.

- Telephone (U.S.A.): 1-800-NICOLET (1-800-642-6538)
- Fax: 1-608-273-6045
- World Wide Web: http://www.nicolet.com
- E-mail: nicinfo@nicolet.com

Conventions used in this manual

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



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

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

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

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

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

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Installing OMNIC

If you purchased your computer from Nicolet, your software is already installed. If you provided your own computer, you will need to install OMNIC on your hard drive. These same instructions can be used should you ever need to reinstall OMNIC.

1. **Start your Windows software**

2. **Insert the CD entitled Disc 1: Software and Libraries (the OMNIC CD) into the drive.**

   The installation starts automatically.

If the installation does not start within 20 seconds, or if you are installing the software from floppy disks, use the Add/Remove Programs dialog box to install OMNIC.

1. **Click the Start button and choose Control Panel from Settings.**

2. **Double-click the Add/Remove Programs icon, and then choose the Install/Uninstall tab in the window.**

3. **Click the Install button and follow the directions to install the OMNIC software.**

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Starting OMNIC

To start OMNIC:

1. **Start your Windows software.**

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

   The OMNIC shortcut is on the Windows desktop.



OMNIC
E.S.P.

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



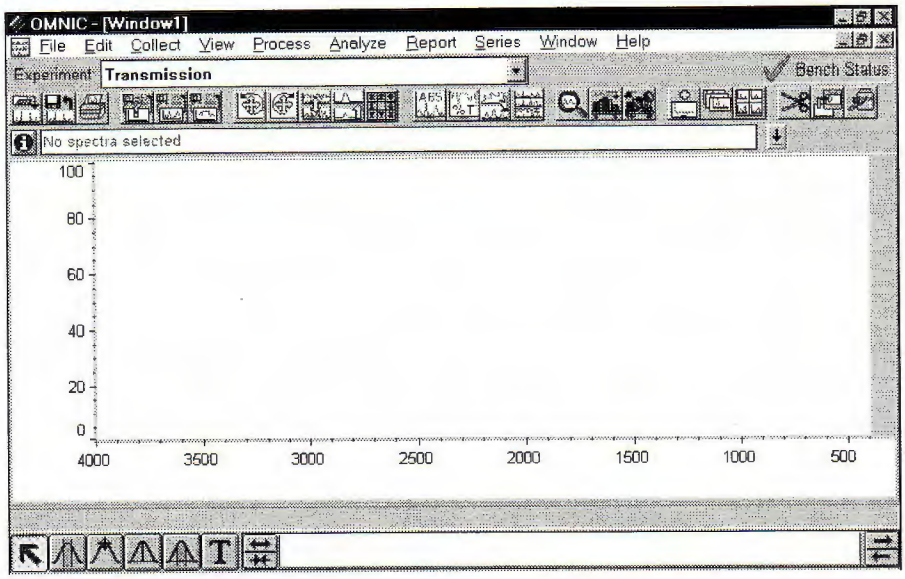
The OMNIC window appears. The OMNIC window is described in the "Getting Started" tutorial in the Help menu.

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

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The OMNIC window

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



Spectral window

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

Menu bar

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

Experiment list box

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

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for any Smart accessory you have installed. By selecting an experiment with this feature, you can quickly set the software parameters for the type of experiment you want to perform. You can see the parameter settings for the selected experiment by using Experiment Setup from the toolbar or from the Collect menu.

Bench status



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

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

Toolbar

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

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.

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Wizards and tutorials

Most of the wizards and tutorials can be accessed through the OMNIC Help menu. Others, like the Avatar Installation Wizard can be accessed using a short cut.

The wizards and tutorials teach you how to do these things:

Avatar Installation Wizard — This tutorial starts automatically whenever you start OMNIC and walks you step-by-step through installing your spectrometer yourself and confirming that the spectrometer is operating properly. Use the check box on the last page of the tutorial if you do not want to see this tutorial each time you start OMNIC. You can start this tutorial at any time by double-clicking the Avatar Installation Wizard short cut.

Getting Started — The "Getting Started" tutorial introduces you to the OMNIC E.S.P. software. This tutorial includes basic information about the OMNIC window, using the toolbar and tool palette, creating and using spectral libraries, creating your own experiment files, and using on-line laboratory notebooks to create and save reports.

Spectrometer Tour — When you finish this tutorial, you will be familiar with all of the components in your spectrometer.

Beginner's Guide to FT-IR — Run this tutorial to learn how an FT-IR spectrometer works and the theory behind FT-IR spectroscopy.

Sampling Techniques — This tutorial helps you choose the best sampling technique for your analysis. It also describes how to install and use Avatar and other Smart Accessories.

Learning OMNIC — Use this tutorial to get information about using various OMNIC features to collect, display and process spectra.

Installing optional hardware — This tutorial contains step-by-step instructions for installing optional hardware and setting up your spectrometer for a variety of experiments. On-line video help is provided for most procedures.

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Replacing parts — Use this tutorial when you want to change replaceable parts. It also includes on-line video help and instructions for maintenance procedures such as cleaning your spectrometer and checking and changing the desiccant and purge filters.

Troubleshooting — 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 outlines the many support, training, and custom application services available from Nicolet. It includes Technical Support telephone and fax numbers, as well as e-mail and web site addresses.

Note You must have the CD entitled Disc 2: Spectrometer Tutorials and Drivers in the computer to use the multi-media capabilities of the Installation Wizard, the Spectrometer Tour or any of the parts replacement or sample handling tutorials. ▲

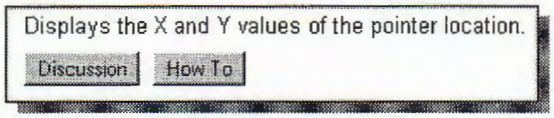
To use a tutorial, point to the Help menu and then choose the desired tutorial from the list that appears. You can access a variety of tutorials from the Learning OMNIC and Choosing a Sampling Technique items in the Help menu. You can also start tutorials from within other parts of the on-line documentation provided with OMNIC.

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OMNIC Help topics

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:

- 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:



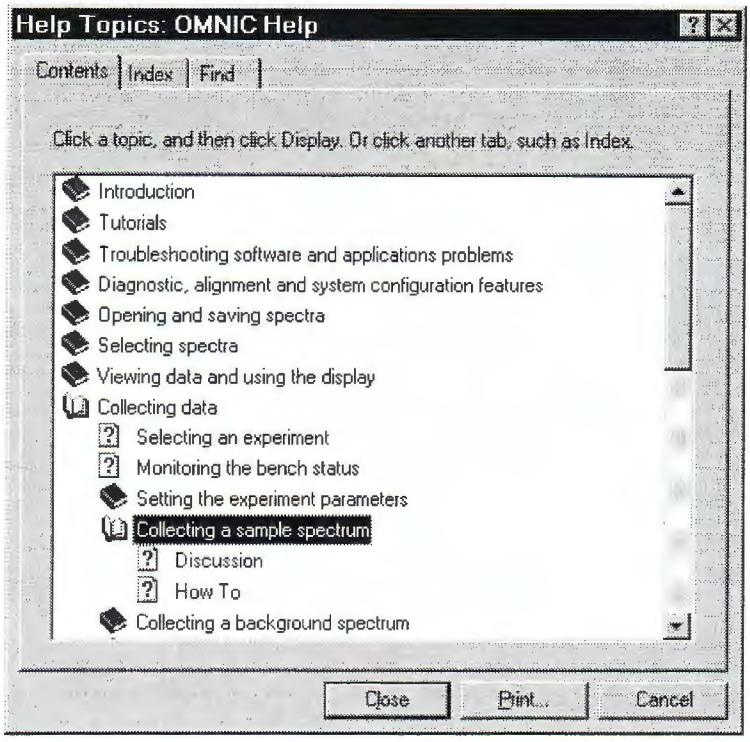
  Click the Discussion button to display a complete discussion of the item (or the dialog box or window that contains the feature). Click the How To button to display a step-by-step procedure for using the item (or the dialog box or window that contains the item).

- You can press the F1 function key 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. Here is an example of the Contents tab displayed in Windows 95 showing the contents of some of the books in the system:

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You can also check parts lists or find other information without using the computer connected to the spectrometer. Insert the Disc 2: Spectrometer Tutorials and Drivers CD into any Windows 95, Windows 98 or NT computer and double-click the icon for the following programs:

P360_ENU.HLP Part numbers and hardware setup and

S360_ENU.EXE Spectrometer tour

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If you purchased EZ OMNIC E.S.P.

The EZ OMNIC E.S.P. version of OMNIC includes the features needed to perform many common spectroscopy tasks. If you purchased EZ OMNIC E.S.P., some of the features described in this manual are not available. In some cases a described command is not in the menu. In other cases certain features do not appear in the dialog boxes for a command. Read and follow the instructions for the features that are available. Here are some other things you should be aware of when using the software:

The toolbar is always displayed when you use EZ OMNIC E.S.P. It provides a convenient way to initiate menu commands, macros and external programs. 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.

If you change the toolbar, you are asked when you exit EZ OMNIC E.S.P. whether to save the changes (the prompt refers to this as saving the "configuration"). Choose Yes if you want the toolbar changes to appear the next time you start OMNIC.

Spectral searches you perform with Search in the Analyze menu (or with the Search button in the Library Setup dialog box) are always carried out using the search expert. The search expert determines the search algorithm to use for the best result and which spectral regions to search. When the search is complete, the library spectra found by the search are displayed along with the search expert's comments.

A special command called Create Library appears in the Analyze menu of EZ OMNIC E.S.P. 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.

While EZ OMNIC E.S.P. cannot be used with Macros\Basic to create new executable macros, you can run existing macros.

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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 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 Avatar 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 E.S.P., 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" and "Spectrometer Tour" tutorials available in the OMNIC Help menu.

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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.

- Cool the detector (if you are using an MCT detector).
- Make sure the spectrometer, computer and printer are turned on and OMNIC is started.
- Check the Power and Scan indicator lights on the spectrometer front panel. The Power light should be on, and the Scan light should be on continuously or flashing. If the lights are not performing in this way, follow the troubleshooting messages that appear on the screen, run the "Troubleshooting" tutorial in the OMNIC Help menu, or see the "Hardware Troubleshooting" chapter of this manual for instructions.
- Check the purge filter and humidity indicator.



For step-by-step instructions for each of these items, run the "Replacing parts" tutorial available in the OMNIC Help menu.

Selecting an experiment

The parameters for spectral data collection are stored in experiment files. You load the parameters you wish use when you select an experiment file from the Experiment drop-down list box below the OMNIC menu bar. A number of experiments are provided with OMNIC, and you can create and save your own.





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



To learn more, see the "Collecting a Spectrum" tutorial. If you need to change a source or detector, see the "Replacing parts" tutorial.

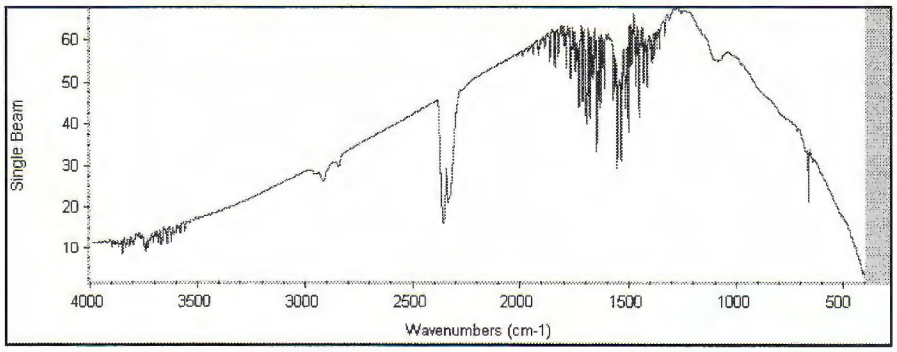
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Note The most commonly used hardware configuration for mid-IR experiments includes a KBr beamsplitter, an Ever-Glo (mid-IR) source and a DTGS detector. You may need to change the settings of the example experiment if your hardware configuration is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

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 background spectrum:



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



Whenever you collect a background spectrum, make sure that the sample compartment is empty You can initiate background data collection at any time using the Collect Background button.

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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 OMNIC Help menu. Then choose the "Removing the Snap-In baseplate" topic from the "Replacing parts" book.

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 using the "Collecting a Spectrum" tutorial available through the Learning OMNIC item in the Help menu.

Follow these steps to collect the sample spectrum:

1. **Select an experiment from the Experiment drop-down list box.**

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



   The Default - Transmission experiment appears in the list. A number of other experiments are included with OMNIC E.S.P. for performing a wide variety of data collections. You can open these experiments by choosing Open in the Experiment Setup dialog box. You can also use Experiment Setup to set up and save your own experiments.

   Select an experiment by clicking it.

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If you select the Default - Transmission experiment, the parameters in the Experiment Setup dialog box are now set correctly for collecting a polystyrene sample spectrum.



You can check the settings of the parameters by choosing Experiment Setup from the toolbar or the Collect menu.



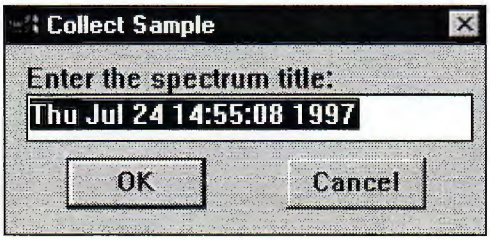
The data collection parameters, along with the other experiment parameters, determine how OMNIC collects background and sample spectra. See the OMNIC Help system for complete information about the parameters.

In the Default - Transmission experiment the Collect Background Before Every Sample option is selected. This option prompts you to collect a background spectrum before you collect a sample spectrum



2. Click the Collect Sample button in the toolbar to begin collecting the sample spectrum.

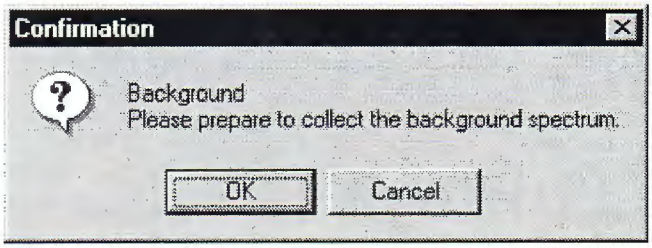
The Collect Sample window appears and then a dialog box showing the default title for the sample spectrum:



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

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



   This means that you need to remove any sample from the sample holder so that the infrared beam path is clear.

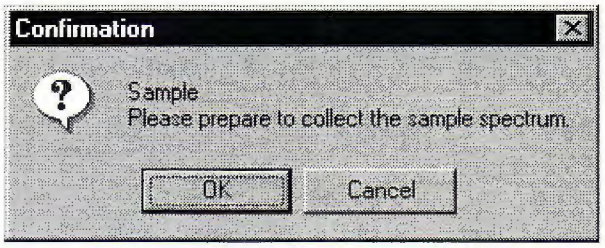
   When you then collect a background spectrum, the result is a measurement of the response of the spectrometer alone; that is, without absorptions due to a sample.

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

   If there is a sample in the sample holder, open the sliding door, remove the sample, close the sliding door, and then choose OK. If your spectrometer is purged, leave the sliding door open about 1 cm (1/4 to 1/2 inch) and wait 1 minute before choosing OK.

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



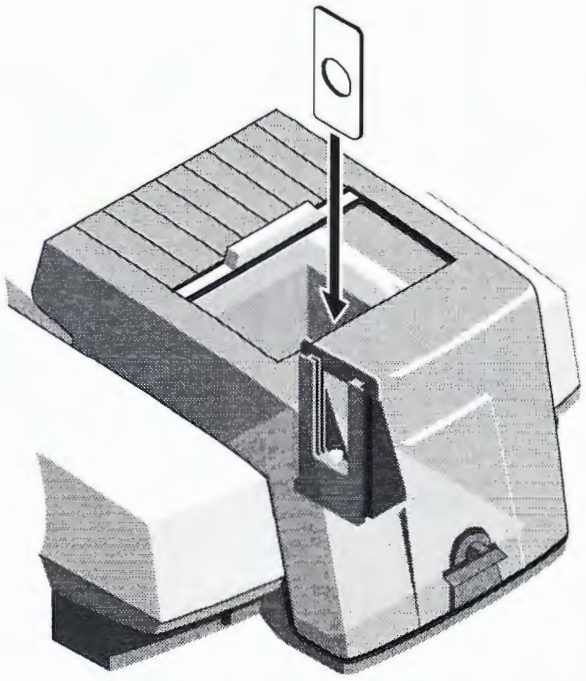
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5. Install the sample.

First open the sliding door.

Next insert the sample into the sample holder. If you are collecting a polystyrene spectrum using the standard samples that came with your spectrometer, insert the 1.5 mil standard.

Then close the sliding door.



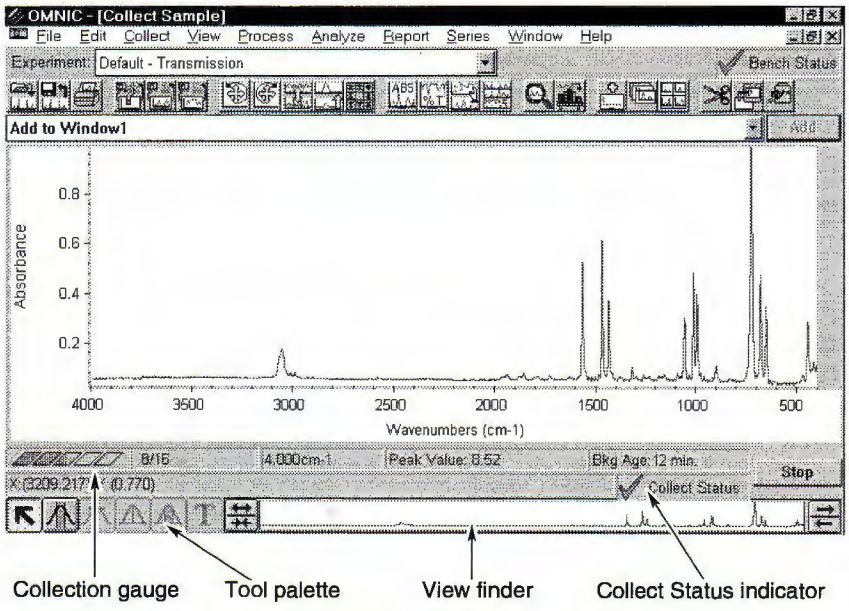
View the "Installing Samples" unit of the "Spectrometer Tour" tutorial for more information about installing samples.

If your spectrometer is equipped with a purge kit, allow 1 minute for the purge to reach equilibrium before going to the next step. If carbon dioxide and water vapor interfere with the spectral data from your sample, you would need to wait 3 to 5 minutes.

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6. Choose OK to start sample data collection.

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



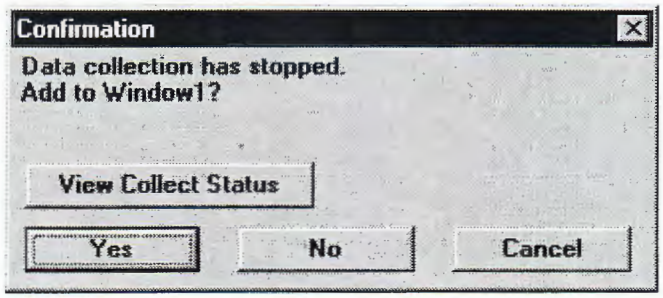
Sample spectrum

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7. **Monitor the status of the data collection.**

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

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

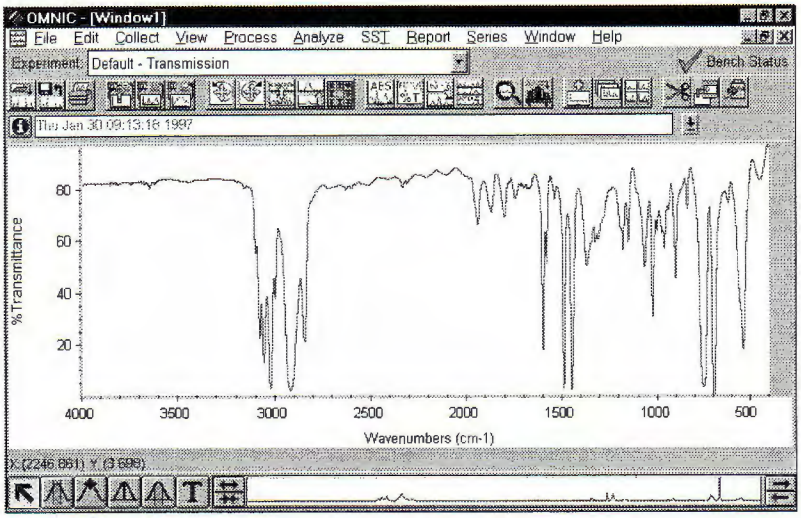


8. **Choose Yes to add the sample spectrum to the spectral window.**

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

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Here is the sample spectrum displayed in the spectral window:



How do I know if my spectral data is good?

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



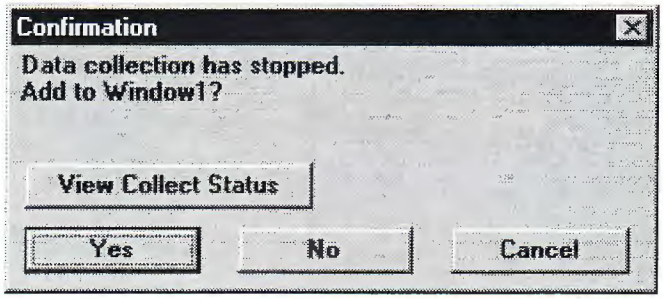
If you ever have a problem with data collection, the Collect Status indicator may change. If the indicator is a yellow circle, the spectrum has failed a spectral quality check (a measured value was not within the allowed range), but it is not serious enough to stop the collection.

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

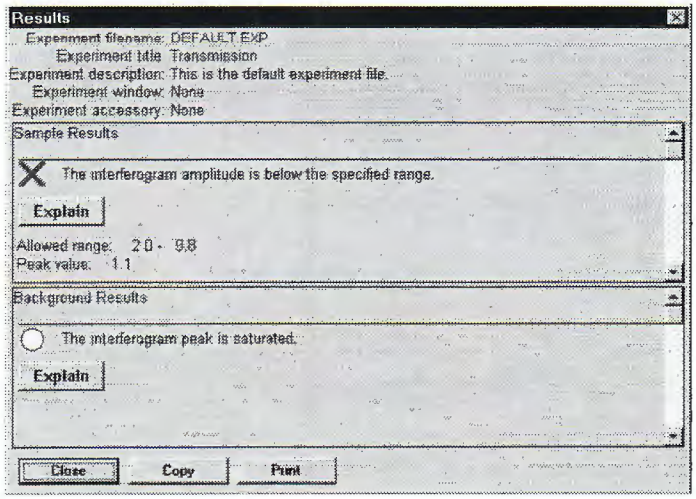
To view information about the collection, including any problems that have occurred, click the indicator during or after the collection, or click the View Collect Status button.

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



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



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Saving the spectrum

You can save your spectrum manually on the hard disk by using either of two commands in the File menu: Save or Save As.

Use Save when you want to save a spectrum on the disk using the current filename and path. In this example you will use Save As to save a spectrum in a file on the disk using a new filename.

Follow these steps to save the spectrum you just collected:

1. **Select the spectrum using the left mouse button.**

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

   The Save As dialog box appears.

3. **Type a descriptive name (for example POLY.SPA) for the spectrum.**

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

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

4. **Choose OK.**

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

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Using Other Basic Features of OMNIC

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

- convert the spectrum's units
- annotate the spectrum
- create and use spectral libraries
- create and view on-line laboratory notebooks, and

Converting a spectrum's units

The spectra you collect using the Default - Transmission experiment are in absorbance units, since many OMNIC data manipulation commands work best on spectra in absorbance units. Often it is useful to convert a spectrum to other units. For this example you will convert the spectrum to % transmittance units.

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



2. **Choose the Transmittance button in the toolbar.**

   You can also choose % Transmittance from the Process menu. The spectrum is converted to % transmittance units.



The toolbar buttons and the Process menu allow you to convert spectra to several other units as well. In the OMNIC Help system Index, find "converting spectrum" and go to the topic discussing the units to convert to.

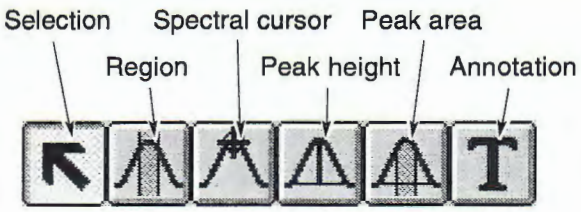


Choose the Absorbance button to return the spectrum to absorbance units so that the spectrum is ready for you to learn to label a peak in the next exercise.

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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; for example, the X and Y values of the pointer location or the limits of the selected spectral region. Here is an example of X and Y values displayed in the readout when the selection tool is selected:

X:(736.294) Y:(1.166)

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



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

   The annotation tool in the palette 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 a pane of a spectral window, the pointer looks like this:

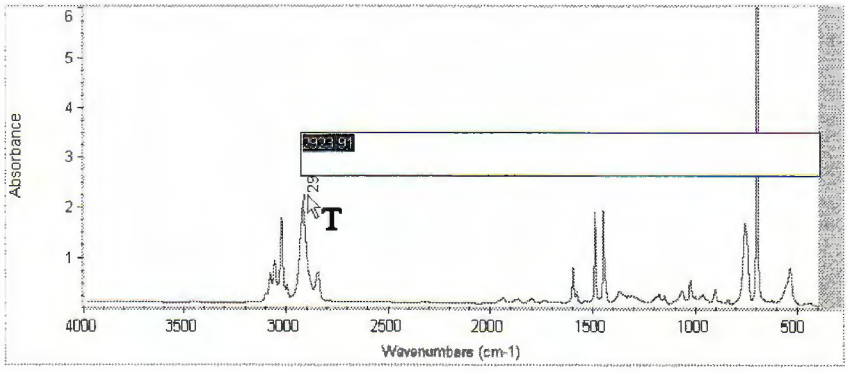


   You can label a peak by clicking above it with the annotation tool. This displays the label text above the peak with a line connecting the label to the peak. The text is selected so that you can immediately edit it. When you press Enter, the label appears in its final form.

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

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

   The label appears:



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

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

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



In the OMNIC Help system Index, find "tool, annotation" and go to the "Annotation tool" topic for more information about 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 E.S.P. allows you to create three different types of spectral libraries.

- Search libraries
- Quality control (QC) libraries
- Scrapbook libraries

Note Scrapbook libraries are not available if you are using EZ OMNIC. ▲

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Searching

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

OMNIC gives you the choice of using the "search expert" to determine how to perform a spectral search and the kinds of search results to display, or specifying the search parameters and results yourself. Unless you have special needs, we suggest that you use the search expert. When a search is complete, the expert displays a 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.



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

Comparing

QC (QC Compare) 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 allows you to maintain reference spectra that reflect variables in or tolerances allowed for your samples. The software then compares your sample spectrum with the reference spectra in each compound type and reports the best compound type match.

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 the OMNIC Help system Index, find "QC comparison" and go to the "Performing a QC comparison" topic if you want more information.

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Browsing

Scrapbook libraries are a convenient place to store and organize your spectra when you are using OMNIC E.S.P. spectroscopy software. You can add any spectrum to a scrapbook library; the resolution and other parameters do not matter.

After adding 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.

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 with EZ OMNIC. ▲



In the OMNIC Help system Index, find "library, searching for text in" and go to the "Searching a library for text" topic if you want more information about organizing sample spectra in scrapbook libraries.

Creating a user library

Both OMNIC E.S.P. and EZ OMNIC E.S.P. include a Library Creation Wizard that 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 are to be performed. The Library Creation Wizard leads you step-by-step through the process.

To access the Library Creation Wizard using OMNIC E.S.P.:

1. **Open Library Manager.**

   Choose Library Manager from the Analyze menu.

2. **Choose Create Library on the Library Names tab.**

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To access the Library Creation Wizard using EZ OMNIC:

Choose Create Library from the Analyze menu.



In the OMNIC Help system Index, find "library,creating" and go to the "Creating a user library" topic if you want more information about creating libraries and using the Library Creation Wizard.

Adding a spectrum to a library

Once you have created a user library, you can use the library to store spectra you 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 collected from one user library into another user library, choose Library Manager from 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 the OMNIC Help system Index, find " adding, spectrum to user library" and go to the "Adding library spectra a user library" topic or the "Adding spectra to a user library (Add to Library)" topic if you want more information about storing spectra in libraries.

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Creating and printing a report

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

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

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

2. **Go to the C:\OMNIC\REPORT directory and select the report template file named SEARCH1.RPT.**

   This file contains a report template specially set up for this procedure. It includes items for the spectral window, spectrum time, title and comments, and search results.

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

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

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

   You can create your own report templates by using the Create button, or you can modify one of the existing templates

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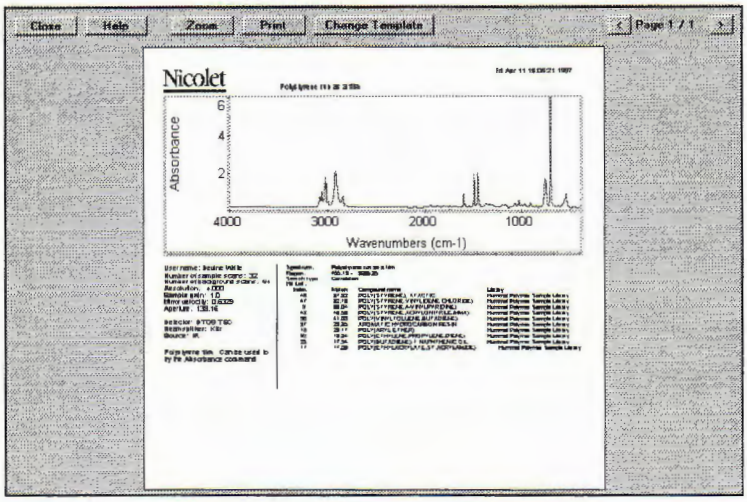
whenever you want to design a new template. Save the template with a new name after you make your changes.



In the OMNIC Help system Index, find "report template, selecting" and go to the "Selecting, editing or creating a report template" topic for more information about using reports.

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

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



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

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

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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.

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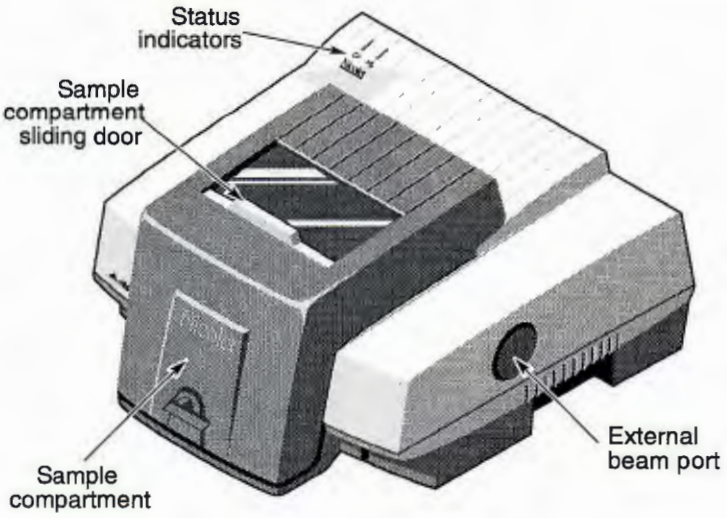
Spectrometer Basics

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

View the "Spectrometer Tour" tutorial for complete descriptions of your spectrometer's internal and external components.

Major spectrometer components

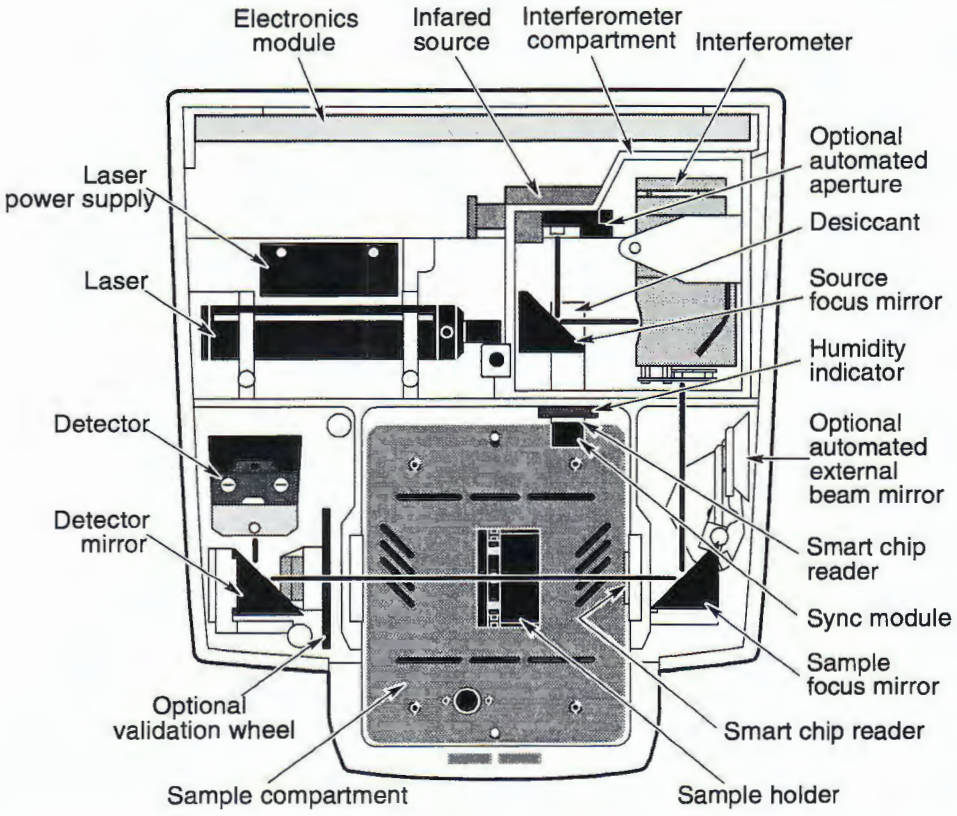
The following illustration shows an Avatar 360 spectrometer from the front.



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What's inside?

The illustration below shows a top view of the optical layout of the Avatar 360 spectrometer with covers removed to reveal components. The solid black line shows the path of the infrared beam.

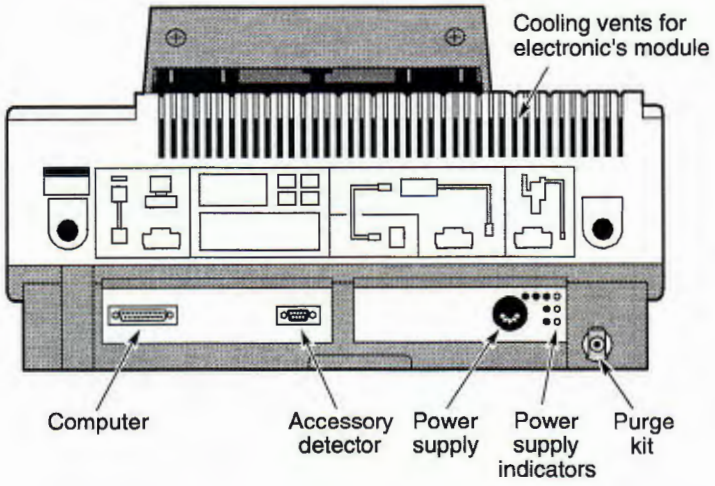


View the "Inside the spectrometer" unit of the "Spectrometer Tour" tutorial for complete descriptions of your spectrometer components.

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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 back panel" unit of the "Spectrometer Tour" tutorial for complete descriptions the rear panel components.

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 Liquid Analysis System.

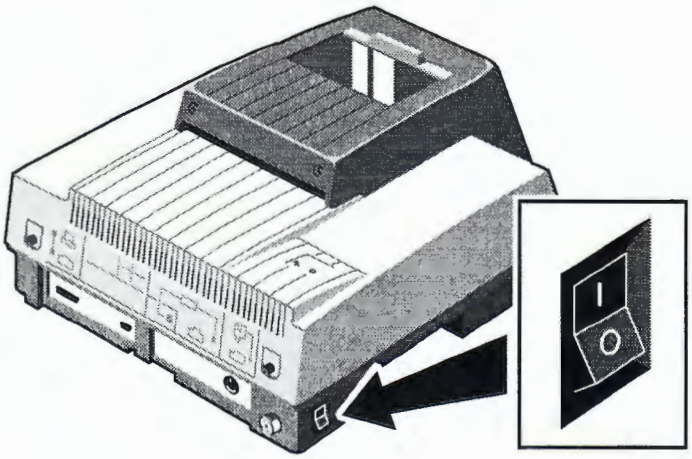
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2. **Turn on the computer and printer.**

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

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

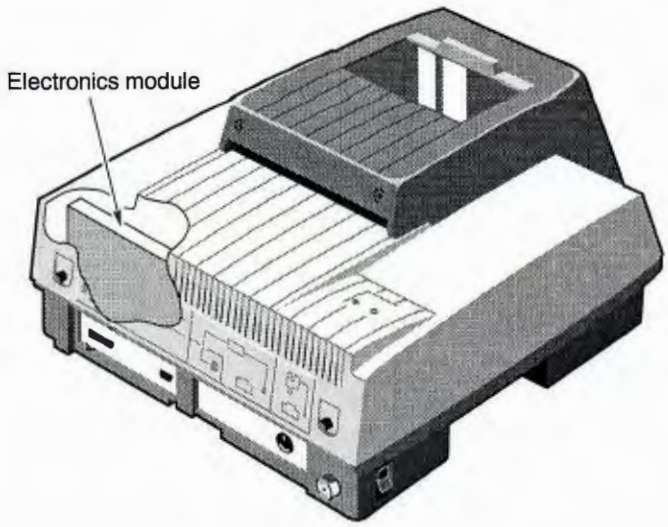
   I = on
   O = off



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

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▲ Caution Never block the cooling vents.



The electronics module inside the spectrometer could overheat. ▲

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

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

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 lighted. You can start your spectroscopy software (OMNIC, EZ OMNIC, or other 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.

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

- Telephone (U.S.A.): 1-800-NICOLET (1-800-642-6538)
- Fax: 1-608-273-6045
- World Wide Web: http://www.nicolet.com
- E-mail: nicinfo@nicolet.com ▲

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More About Your Spectrometer

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

Using sources and detectors

The Avatar 360 spectrometer is available with a single internal source, a single internal detector, and a permanently installed beamsplitter. The source and the detector can be changed to allow you to study a broader spectral range with one instrument. However, not all beamsplitters, detectors, and sources can be used together. Some detectors can accommodate only a portion of the energy from the source and may require installing an energy filter. Be sure to select a detector-source combination that is compatible with the beamsplitter that is installed in the spectrometer.



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



In the OMNIC Help system Index, find "source" and go to the "Specifying the source type" topic for instructions on using different sources in your spectrometer.

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Selecting the right detector

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

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

Light Range	*Beamsplitter*	*Detector*	*Spectral Range (cm^{-1})*	*Source*
near-IR	CaF_2	MCT-A‡	11,700 - 1,200*	Ever-Glo, white light
mid-IR	KBr	DTGS-KBr	7,400 - 350	Ever-Glo
		MCT-A‡	7,400 - 600	Ever-Glo

Notes:

* This spectral range reflects the combination of the ranges of the Ever-Glo and white light sources, as well as the limits of the beamsplitter-detector combination. The range achieved using one of these sources will not be as broad as the total range shown.

‡ These detectors 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 are photometrically accurate. 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.

If you are studying samples that produce tiny spectral peaks, have weak spectral features, or if you are looking for small changes in your samples, you want to be sure that the signal-to-noise ratio is

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high enough so that you can 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, by building vibrations, by light source fluctuations, and other such sources.

Avatar 360 detectors can be optimized 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 (using a larger Resolution setting).

Another method is to use an energy screen that transmits more light (or no screen at all). In this case, the resulting spectrum might be distorted and accuracy and stability could be reduced. Checking the single-beam baseline in the region below the low-end cutoff will give you a rough idea of how much distortion is occurring. If the distance from the baseline to 0 is more than 15% of the spectrum's maximum intensity value, you may have difficulty reproducing the results. Screens generally are not needed for DTGS detectors.

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



See "Setting up for experiments" available through Installing Hardware in the Help menu for instructions for installing filters and energy screens.

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Improving linearity and photometric accuracy

Some detectors (including PbSe and 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.

Look at a single-beam spectrum in the low-end region around 600 to 350 cm^{-1}. You should see a straight line very near 0. As a rule of thumb, the distance from 0 to the baseline should be less than 1% of the spectrum's maximum intensity value. If the detector is saturated, you will see false energy in the low-end region. The baseline might be far above zero.

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

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

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

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To solve these problems, Avatar 360 spectrometers allow the following options for modifying the infrared beam:

- Install a bandwidth-limiting filter.
- Install an energy screen.



See "Setting up for experiments" available through Installing Hardware in the Help menu for instructions for installing filters and energy screens.

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

When to use bandwidth-limiting filters

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



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

When to use energy screens

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

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.

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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.



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

About the moving mirror velocity

Several moving mirror velocities are available for Avatar spectrometers. 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.

For DTGS detectors, the Velocity parameter values should be 0.63 or less. Higher velocities cause a decrease in the detector's sensitivity and increase the noise in your spectrum. To specify the velocity and spectral range, use the Velocity and Spectral Range settings on the Bench tab in the Experiment Setup dialog box. To specify the resolution, use the Resolution setting on the Bench tab.

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Accessories You Can Buy and How to Install Them

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

Avatar Smart Accessories

A variety of "Smart" accessories have been designed specifically for your Avatar spectrometer.

The new Avatar Smart Accessories take a generational leap forward to provide easy sample preparation and complete, reliable sampling performance. The Avatar system uses E.S.P. technology to identify each Avatar accessory as soon as it is installed. When you "snap in" an Avatar Smart Accessory, you are ready to collect data. No more time is wasted aligning accessories and setting parameter files.

Avatar Multi-Bounce HATR — This attenuated total reflection spectroscopy accessory is ideal for rapid quantitative and qualitative analyses, since sample preparation is usually not necessary. It is well suited for a range of solids and liquids. Analyzing liquids, pastes, gels, films, and soft powders is effortless. This accessory is available with a Trough Plate Kit for analyzing liquids, pastes and gels; a Flat Plate Kit for analyzing films and coatings on flat samples; or a Combination Kit for a variety of liquid and solid samples. The Trough Plate and Combination Kits include a volatile liquid cover and a powder press. Zinc selenide (ZnSe) is the standard crystal material for this accessory. Germanium (Ge) crystals are available as an option for measuring samples with a high refractive index.

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Avatar Single Bounce HATR — This attenuated total reflection spectroscopy accessory is recommended for analyzing samples with strongly absorbing spectral peaks. It is also useful for analyzing discreet areas (8 mm or larger) such as a spot on a film. It is well suited for analyzing neat solvents, aqueous solutions, pastes, gels, films, and hard samples. The shorter, single-reflection pathlength produces absorbance values that are within the linearity of the FT-IR technique and therefore permits more complete and accurate spectral subtractions. This high quality subtracted data can be readily searched against library data bases. Both ZnSe and Ge crystals are available for this accessory.

Avatar Diffuse Reflectance — The Avatar Diffuse Reflectance accessory is highly effective at maximizing diffusely scattered radiation, while minimizing specular reflected radiation (a source of spectral interference). Samples can be analyzed as is, with a slight amount of grinding, or by grinding and mixing with potassium bromide (KBr). The technique is applicable for both organic and inorganic materials. The kit includes a Si-Carb™ sampling tool (for the analysis of solid materials such as paint chips and any inflexible sample that can be abraded with silicon carbide paper) two sample slides, adhesive-backed silicon carbide disks, and pre-measured and sealed KBr packets.



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

Other sampling accessories for different applications

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

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Most accessories fit into the sample compartment, but some require separate housing and optics. Nicolet offers microscopes and liquid analysis systems with the Avatar 360.

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

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

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

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

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

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

IR microscopes — Nicolet offers microscopes that attach directly to the spectrometer. The microscopes provide fast, nondestructive

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microanalysis with minimal sample preparation and alignment. The beam path is switched from the spectrometer to the microscope module through the OMNIC software.

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

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

Transmission — Transmission is the oldest and most efficient sampling technique in FT-IR spectroscopy and can be used for sampling liquids, gases or solids. A variety of cells and sample holders are available for transmission analysis. All can be mounted in the spectrometer sample compartment.

The standard transmission baseplate is an E.S.P. accessory. E.S.P. accessories are automatically recognized by the Avatar 360 E.S.P. spectrometer and OMNIC E.S.P. software. The system automatically selects the correct operating parameters for the system when the Transmission E.S.P. baseplate is installed. Also, a series of spectral quality checks are performed to ensure that the accessory is installed and operating correctly.

Validation wheel — The validation wheel is used with Nicolet's System Validation software to validate the performance of the spectrometer. The wheel automatically moves standard samples into the beam path at the appropriate times during the validation procedure. You can choose a validation wheel permanently installed

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in the detector compartment, or one that mounts in the sample compartment.



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

System accessories

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

Automated aperture — This option allows you to perform high resolution (0.5 cm^{-1}) experiments.

Automated external beam mirror — If you have a microscope, Liquid Analysis System or other accessory with an external detector, this option is required. It directs the IR beam out the port on the side of the spectrometer to the accessory whenever you select it.

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

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

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 Nicolet warranty.

Pure air dryer — Nicolet offers dry-air systems. If you have difficulty controlling moisture in your laboratory, the pure air dryer provides additional protection for the hygroscopic elements of your

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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, Nicolet offers several purge gas generators. These systems include an air compressor and an air dryer.

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

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

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

Collecting spectra

How do I set the software for collecting spectra?



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



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

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

How do I collect a spectrum?



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



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

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

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



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

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



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

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

What does gain do?

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



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

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

When should I save interferograms with my spectra?

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Save interferograms if you think you may want to restore the original data after it has been processed or if you want to keep an archive of your raw data. This setting increases the size of files stored on your hard disk.



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

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

What does the Collect Sample window show?

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



View the "Collecting the Spectrum of a Sample" unit of the "Collecting a Spectrum" tutorial.

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

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.

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OMNIC offers four categories of spectral quality checks:

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

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



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

Converting spectra to other units

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

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

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

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

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

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

In the OMNIC Help system Index...

- Find "absorbance" and go to the "Converting spectra to absorbance" topic.
- Find "transmittance (%)" and go to the "Converting spectra to % transmittance" topic.
- Find "Kubelka-Munk units" and go to the "Kubelka-Munk units" topic.
- Find "reflectance (%)" and go to the "% Reflectance units" topic.
- Find "log (1/R) units" and go to the "Log (1/R) units" topic.

Using spectral libraries

How do I search a spectral library?

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



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

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

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

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

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

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



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

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



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

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



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

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



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

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

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

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



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

How do I create a spectral library?

For OMNIC E.S.P. users, use the Create Library button on the Library Names tab of Library Manager to create a user library.

For EZ OMNIC E.S.P. users, use Create Library from the Analyze menu.

When you create a library, you determine the kinds of information that will be saved with it. Once the library is created use Add To Library from the Analyze menu to put your spectra into it.



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

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

Locate and select the spectrum in Library Manager and then click the Add To Window button, or go to the Library Spectra tab of Library Manager, display the desired spectrum on the tab and then double-click the spectrum.



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

How can I find a compound in a commercial library?

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



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

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



In the OMNIC Help system Index, find "extended search" and go to the "Using extended search" topic.

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

Use the Collect Spectrum button on the Library Names tab of Library Manager to collect a spectrum and add it to a user library.

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The software automatically sets the experiment parameters (for example, Resolution) so that the spectrum will be compatible with the selected library. This allows you to collect and add a compatible spectrum in one step instead of three (using Experiment Setup to set the parameters, Collect Sample to collect the spectrum and Add To Library to add the spectrum to the library).



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

What does the search expert do?

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

Opening, saving and deleting spectra

How do I open a stored spectrum?

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



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

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How can I automatically save my collected spectra?



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



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

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

Where should I save my spectra?

You have several options for saving spectra; you may choose to use more than one. For a permanent record of the spectrum and any other information you want to record, use a report notebook.



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

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



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

We recommend that you create descriptively named folders (directories) on your hard disk for different categories of spectra. For example, you could have a folder for each project you are working on, for each of your clients, for each laboratory application,

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or for each sample type. See your Windows documentation for information about creating directories. You can specify which folder to use when you use Save or Save As in the File menu to save spectra. This will make it easier to find a spectrum in a particular category when you use Open in the File menu to open a spectrum.



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

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

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



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

How can I delete stored spectra?

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



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

Can I delete an entry from a report notebook?

No. OMNIC's report notebooks are similar to traditional laboratory notebooks in that information you add to them becomes part of the permanent record of your work. You can delete an entire notebook, however, by deleting the entire notebook file. Choose Delete Files

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

Printing

How can I specify a printer for printing information?

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



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

How can I create and print reports of my work?

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



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

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



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

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How can I preview spectra or other information before printing?

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



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

Displaying spectra

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

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



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

How can I specify colors for displaying spectra?

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



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

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



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

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

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



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

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

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

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

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

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

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

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



In the OMNIC Help system Index...

- For information about Full Scale or Automatic Full Scale, find "displaying, spectra" and go to the "Displaying spectra full scale" topic or "Displaying spectra full scale automatically" topic.
- For information about Common Scale, find "displaying, spectra" and go to the "Displaying spectra using the same Y-axis" topic.
- For information about Match Scale, find "displaying, spectra" and go to the "Matching the Y scale of a spectrum" topic.
- For information about Offset Scale, find "displaying, spectra" and go to the "Displaying spectra vertically offset" topic.

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



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



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

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



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

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



Use the selection tool to drag the spectrum up or down.

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



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

How can I move a spectrum into another spectral window?



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

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

How can I move a stacked spectrum into another pane?



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



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

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



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



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

How can I find the height of a peak?



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



In the OMNIC Help system Index, find "Peak, height" and go to the "Peak height tool" topic.

How can I find the area of a peak?



Use the peak area tool to drag across the peak. Then drag the baseline handles to adjust the baseline used for the measurement.

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The corrected (measured above the baseline) and uncorrected area values appear in the readout above the palette.



In the OMNIC Help system Index, find "Peak, area" and go to the "Peak area tool" topic.

Correcting spectra

Should I correct the baseline of my spectrum?

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

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



View the "Common Problems" unit of the "Collecting a Spectrum" tutorial.

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

Subtracting, adding, multiplying and dividing spectra

How can I subtract a spectrum from another spectrum?

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

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

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Note Subtract is available in the Process menu only when two spectra are selected. ▲

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



In the OMNIC Help system Index, find "subtracting, spectra" and go to the "Subtracting spectra" topic.

What should I use subtraction for?

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

Spectral subtraction is useful in a variety of situations. Here are some examples:

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

What other arithmetic operations can I perform on my spectra?

You can manipulate your spectra using any of the common arithmetic operations. Use Spectral Math in the Process menu to perform these operations on one or two selected spectra. You

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specify the operations to perform by typing a sequence of mathematical symbols and numbers. The software performs the operations on the Y values of the data points in the spectrum or spectra and then displays the result spectrum.

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



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

Customizing OMNIC

How can I customize my OMNIC software?

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



View the "Preparing the Software" unit of the "Collecting a Spectrum" tutorial.

In the OMNIC Help system Index...

- Find "options" and go to the "Customizing OMNIC by setting options" topic.
- Find "customizing, menu" and go to the "Customizing a menu" topic.
- Find "customizing, toolbar" and go to the "Customizing a toolbar" topic.
- Find "saving, configuration" and go to the "Saving a configuration" topic.
- Find "opening, configuration" and go to the 'Opening a configuration" topic.

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Other questions

How can I find and label peaks in spectra?

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



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



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

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



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



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

How can I select a spectral region for an operation?



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



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

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

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



In the OMNIC Help system Index, find "collection and processing information" and go to the "Collection and processing information" topic.
If you want this kind of information displayed in a spectrum's pane, choose Display Setup from the View menu, turn on Sampling Information and then specify the types of information you want displayed by turning on options in the Sampling Information box.



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

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

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



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

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Quick Answers to Your Questions About Using the Spectrometer

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

When do I need to remove the spectrometer cover?

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



See "Removing the cover" available through Replacing Parts in the Help menu for instructions for removing the cover.

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 first. ▲

When should I align the spectrometer?

Align the spectrometer after you replace the laser or move the spectrometer. It is also a good idea to align the spectrometer if the signal intensity has dropped significantly from its usual level.

Note Turn on the spectrometer and leave it on for at least an hour before you align it. This allows the spectrometer to reach thermal equilibrium. ▲



View the "Testing Performance" unit of the "Collecting a Spectrum" tutorial for information about when to align the spectrometer.

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In the OMNIC Help system Index, find "aligning, spectrometer" and go to the "Aligning the spectrometer" topic for information about performing an automatic alignment.

Does my detector need to be cooled with liquid nitrogen?

Most detectors (including the standard DTGS detector) do not need to be cooled. Detectors that have a dewar need to be cooled. Dewar detectors are insulated metal cylinders with a hole in the top. These include MCT detectors.

If during a work session you find that the signal intensity from your cooled detector is decreasing, it may need to be refilled with liquid nitrogen.

When should I change the desiccant?

When the desiccant indicator at the rear of the sample compartment turns light purple, change the desiccant cartridge. Do not discard the spent cartridge. It can be baked out, stored in a desiccator, and used the next time you need to change the cartridge.

You should check the indicator every two months, more often if your laboratory is not air conditioned.



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

Which source should I use?

Use the source that is appropriate for the spectral range of your experiment (determined by the ranges of the beamsplitter and

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detector). Nicolet offers a mid-IR source (Ever-Glo) and a near-IR source (white light).



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

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

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 is displayed on your screen.



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

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

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

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information about ordering replacement parts. See the "Service and Maintenance" chapter of this manual for more information.



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

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

In most cases, no. If you are using a highly sensitive detector such as a PbSe or MCT-A detector and your experiment deals with information from a broad range of frequencies, use an energy screen to prevent the detector from becoming saturated or producing a distorted signal.



See "Setting up for experiments" available through Installing Hardware in the Help menu for information about installing energy screens.

Do I need to use a bandwidth-limiting filter?

In most cases, no. If you are using a highly sensitive detector such as a PbSe or 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.



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

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Service and Maintenance

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

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

- Telephone (U.S.A.): 1-800-NICOLET (1-800-642-6538)
- Fax: 1-608-273-6045
- World Wide Web: http://www.nicolet.com
- E-mail: nicinfo@nicolet.com ▲



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

Running diagnostic tests

If your system is not performing properly, you can use the Diagnostic tab in the Experiment Setup dialog box to check the performance of spectrometer components. You should run these diagnostic tests if you have problems with your spectrometer to determine the source of the problem.

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To run the spectrometer diagnostic tests:

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

   Remove any samples and sampling accessories.



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

3. **Click the Diagnostic tab.**

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

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

   When you click one of the indicators, a dialog box appears showing information about the status of the component. If the operating values for the component are within proper limits, a check mark appears in the Status column. If the value is outside the acceptable range, an X appears in the Status column.

   When you are finished viewing the information, choose OK.

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Service

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

Note The diagnostics software will alert you to failing components. See the troubleshooting information available in the Help menu for instructions on diagnosing spectrometer problems, ordering parts and replacing parts. ▲

If the source, laser module, electronics module or power supply must be replaced, refer to the replacement parts list available through Replacing Parts in the Help menu. Call 1-800-NICOLET (1-800-642-6538) or 1-608-276-6373 to order the replacement assembly. If you are outside the U.S., contact your local Nicolet office. Telephone numbers for all Nicolet Customer Support offices are provided with the documentation with your spectrometer.

Maintenance

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



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

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Aligning the spectrometer

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

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

Follow these steps:

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

   The beam path must be clear during alignment.



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

   The Experiment Setup dialog box appears.

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

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

   Do not use Autogain.



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

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

If you want to hear a tone whose pitch indicates the signal intensity, turn on the Tone check box on the Bench tab. The

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tone reaches its highest pitch when the signal is maximized.

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

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

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

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

Aligning an accessory

You can also align accessories that mount inside a sample compartment. (This does not include Smart accessories, which do not require alignment.) First align the spectrometer, 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 and diffuse reflection accessories typically use a Gain setting of 2 or 4.

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

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

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

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

Performance test

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

Follow these steps to conduct a performance test:

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

   Remove any samples and sampling accessories.

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

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

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

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

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

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

Note If the noise readings are greater than normal or have changed significantly, align the spectrometer and check the purge or desiccant. A gradual increase in noise as the spectrometer ages is normal. If the noise level suddenly increases to twice its normal level or higher, a component may be defective; call the Nicolet Customer Support Department for assistance. Outside the U.S.A., call your local service representative. Telephone numbers for all Nicolet Customer Support offices are provided with OMNIC Help. ▲

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

Checking the purge

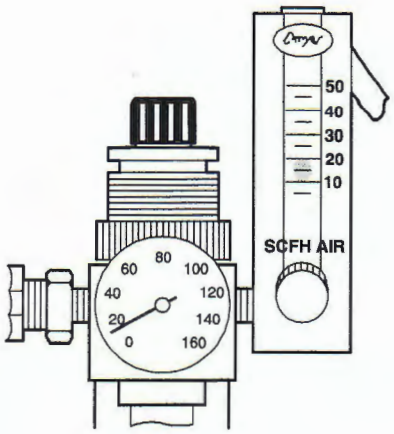
If your spectrometer is equipped with an optional purge kit, make sure the pressure regulator is set between 10 and 20 pounds per square inch (psi) and the flowmeter is set to 15 standard cubic feet per hour (scfh).

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

⚠ Warning Never use a flammable gas to purge the spectrometer. The purge gas must be free of moisture, oil, carbon dioxide and other reactive or infrared-absorbing materials. We recommend using dry air or nitrogen. Using other gases to purge your spectrometer, including inert gases such as argon (AR), can damage your spectrometer. ▲

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.

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Choose Installing Hardware from the OMNIC Help menu and view the tutorials 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.

Cooling a detector

Standard DTGS detectors do not need cooling. Some optional detectors, such as an MCT detector, require cooling with liquid nitrogen.

Choose Installing Hardware from the OMNIC Help menu and view the "Cooling a detector" tutorial in the "Installing hardware" book for information about how to cool an MCT detector.

Warning Liquid nitrogen is extremely cold and therefore potentially hazardous. Avoid contact with skin. Wear protective clothing and follow standard laboratory safety practices to prevent injury. ▲

After you fill the detector dewar with liquid nitrogen, allow the detector to cool at least 20 minutes before collecting spectra.

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Troubleshooting Software Problems

OMNIC E.S.P. automatically and continuously checks the status of your system. If a problem is found, a message automatically appears allowing access to more information. This chapter lists some simple troubleshooting measures you can take to solve software problems with OMNIC E.S.P. For more information about troubleshooting, consult the OMNIC on-line Help system.

What hardware and software do I need?

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

- Intel® Pentium® processor with 100 MHz or greater clock speed.
- At least 16 megabytes of random access memory (RAM).
- The capability of displaying at least 256 colors.
- Hard disk size of at least 1.0 gigabyte.
- Quad speed CD-ROM drive.
- A 1.44-megabyte floppy disk drive for 3.5-inch floppy disks.
- A 15-inch SVGA monitor with 800 by 600 resolution.
- A keyboard and serial, bus, or PS/2®-style mouse.
- A 16-bit Sound Blaster-compatible sound card.
- Two serial ports (if you plan to use a Plus™ 2 liquid analysis system).
- Two ECP bidirectional parallel ports.
- Three ISA/PCI slots.
- *For OMNIC version 5.0 or greater*
  Windows 95, Windows 98, or Windows NT version 4.0 or greater.
  For OMNIC version 4.xx
  Windows 95, Windows 98, or Windows NT version 3.51 or greater
  (NT systems can be used for workstations only).

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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 the quantitative analysis method using Quant Setup in the Analyze menu. Select a single spectrum. Select an appropriate method for the selected spectrum.
OMNIC needs to be restored after a system crash or a message states that OMNIC cannot start or will no longer run.	There is not enough memory. There is another system problem.	Make sure OMNIC has enough memory. Quit other programs to free memory for OMNIC. Restart Windows. Run the SCANDISK utility included with your Windows software. Restart OMNIC. If OMNIC does not start, reinstall OMNIC.
Libraries created with a previous version of OMNIC are not listed in the Library Setup dialog box.	The libraries are not in one of the directories listed in the dialog box (typically OMNIC\LIBS).	Use the Add Directory button on the Search Libraries tab to add the OMNIC\SEARCH44 directory and any other directories you are using to store libraries.

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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.	Collect the spectrum at the same resolution as the library (first set Resolution on the Collect tab of the Experiment Setup dialog box), and then add it to the library.
	The spectral range of the spectrum does not match the spectral range of the library.	Collect the spectrum at the same spectral range as the library (first set Spectral Range Saved on the Bench tab of the Experiment Setup dialog box) and then add it to the library.
	The spectrum is a commercially collected reference spectrum.	Only spectrum 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 not 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 the 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.

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Troubleshooting Hardware Problems



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

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

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



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 a cooled detector.	The insulating vacuum chamber surrounding the dewar has begun to leak.	If you suspect that your detector has a vacuum leak, choose Troubleshooting from the OMNIC Help menu and choose the MCT detector is warm topic from the General Troubleshooting help book.

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Problem	Possible Cause	Solution
The indicators on the front panel 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 that the lock ring is tightened finger-tight.
	The spectrometer is not plugged in.	Make sure that 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 that the power cord is appropriate for your AC power source. Choose Replacing Parts from the OMNIC Help menu 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. Choose Replacing Parts from the OMNIC Help menu for power cord descriptions and part number information.
	The power cable or power supply is defective.	Check the three power LEDs (next to the power connector on the rear panel). All the LEDs light when the power supply is working properly. If necessary, Replace the power supply. Call Nicolet to order a replacement part. Choose Replacing Parts from the OMNIC Help menu for part number information.

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Problem	Possible Cause	Solution
Data is not displayed during data 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. Use the Align button on the Diagnostic tab of the Experiment Setup dialog box.
	The laser is not functioning.	Check the laser indicator on the Diagnostic tab in Experiment Setup. Replace the laser if necessary.
The Scan indicator does not flash.	The spectrometer is turned off.	Turn on the spectrometer.
	Spectroscopy software has not been started.	Double-click the OMNIC or EZ OMNIC shortcut to start the software.
	No data has been collected for an hour or more and the spectrometer is in "stand-by" mode.	This is normal. The system will begin scanning when you use OMNIC to collect background or sample data.
	The spectrometer is out of alignment.	Align the spectrometer. Use the Align button on the Diagnostic tab in 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 power-up diagnostics finish. Then turn on the computer and restart OMNIC.

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Problem	Possible Cause	Solution
An error message appears when you try to scan.	The light source is not working.	Check the source indicator on the Diagnostics tab in Experiment setup. If necessary replace the source.
	An optional cooled detector is not cooled.	If you are using an optional cooled detector, check and cool the detector.
	The interferogram is not located at 1024 ±16 data points on the Bench tab in the Experiment Setup dialog box.	Align the spectrometer. If the interferogram is still not located correctly, call Nicolet for service.
	The beam path is blocked.	Remove the obstruction.
	The data cable between the spectrometer and computer is not properly connected.	Turn off the spectrometer power and check the data cable connections. Also make sure that the parallel port is in ECP mode.
The signal intensity is low in the mid-IR range.	The optional automated aperture is set incorrectly.	Check the Aperture parameter on the Bench tab in the Experiment Setup dialog box. For DTGS detectors set the aperture to 100; for MCT-A detectors, set it to 10.
	The source is glowing unevenly.	Check the source indicator on the Diagnostic tab in the Experiment Setup dialog box. Order a replacement if needed.
The signal intensity is low, there are frequent interferometer scan restarts (verified by intermittent flashing of the Scan indicator) and the spectrometer alignment fails.	The spectrometer is out of alignment.	Align the spectrometer. Use the Align button on the Diagnostic tab in the Experiment Setup dialog box.
	The beamsplitter is fogged.	Check the laser signals by clicking the laser indicator on the Diagnostic tab in the Experiment Setup dialog box. If you suspect the beamsplitter is fogged, call Nicolet for service.

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Problem	Possible Cause	Solution
The system scans but gives a very low signal intensity.	The spectrometer is out of alignment.	Align the spectrometer. Use the Align button on the Diagnostic tab in the Experiment Setup dialog box.
	The moving mirror velocity is set too high.	For DTGS detectors, reduce the velocity parameter on the Bench tab in the Experiment Setup dialog to 0.63 or less.
	There is no interferogram.	Click the source indicator on the Diagnostic tab in the Experiment Setup dialog box to check the source current and voltage. If the source indicator is on, check the interferogram on the Bench tab in the Experiment Setup dialog box; if the interferogram is not present, check the beam path and detector.
	The optional automated aperture is set incorrectly.	Check the Aperture parameter on the Bench tab in the Experiment Setup dialog box. For an MCT-A detector, set Aperture to 10. For a DTGS detector, set Aperture to 100.
	A non-Avatar sampling accessory is not aligned.	Align the accessory. Use the instructions that were included with the accessory.
The baseline is not stable.	The purge rate is too high.	Lower the purge rate until the baseline is stable. The flowmeter should be set to 15 scfh.
	The spectrometer is out of alignment.	Align the spectrometer. Use the Align button on the Diagnostic tab in the Experiment Setup dialog box.
	The spectrometer cover was recently opened.	Allow the spectrometer to purge for 3 to 5 minutes after the cover is closed.

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Problem	Possible Cause	Solution
Unable to collect data message appears when you start OMNIC.	The printer is using the parallel port for printing.	Wait until the printer is finished and then begin your data collection. The spectrometer cannot collect data while the printer is printing.
	The spectrometer is turned off.	Turn on the spectrometer and wait until the power-up diagnostics finish before restarting OMNIC.
	The data cable is loose, disconnected, or damaged.	Shut down the computer and turn the spectrometer off. 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 power-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 Nicolet for service.

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Problem	Possible Cause	Solution
The spectrometer temperature is out of specification	The vents on the back of the spectrometer are blocked.	Check the cooling vents. Remove any obstructions. Always maintain 30 cm (12 in) of clearance behind the spectrometer.
	There is not enough clearance above the spectrometer.	Remove any items stacked on the spectrometer. Always maintain 45 cm (18 in) of clearance above the spectrometer.
	The ambient temperature in your lab may be too high.	The ambient temperature should be between 16° and 27°C (60° and 80°F).
	A component failed.	Contact Nicolet for service.
The laser is off.	The laser cable is not seated properly.	Turn off the spectrometer and then remove the spectrometer cover to check the cable. See Troubleshooting in the OMNIC Help menu for instructions.
	The laser or the electronics module is defective.	Check the laser status on the Diagnostic tab in theExperiment Setup dialog box. If there is a slash through the laser indicator, click the indicator. If the laser frequency is outside the specified range, replace the electronics module. Choose Replacing Parts from the OMNIC Help menu and use the "Replacing the electronics module" tutorial to find the part number, ordering and installation instructions. If the laser voltage or current are outside the specified range, replace the laser. Choose Replacing Parts from the OMNIC Help menu and use the "Replacing the laser" tutorial to find the part number, ordering and installation instructions.

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Bench Diagnostics

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

You can use the Bench Diagnostics program to:

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

Follow these steps to run the Bench Diagnostics:

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

   Remove any samples and sampling accessories.

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

   Choose Advanced Diagnostics from the Collect menu, or click the Start button, and then choose the Bench Diagnostics icon in the OMNIC E.S.P. folder. Some of the advanced features of the program, including the Performance Test, are not available if you run the diagnostics from OMNIC.

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

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



Click this button to return to the previous window.



Click this button to return to the main Diagnostics window.

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

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Declaration of Conformity

Model: Avatar™ 360

This product complies with the following European Union Directives:

Electromagnetic Compatibility, 89/336/EEC as amended by 92/31/EEC and 92/68/EEC

Low Voltage, 73/23/EEC as amended by 92/68/EEC

The following standards were used to verify compliance with the Directives:

EN 50082-1: 1992, EN 50081-1: 1992, EN 55011: 1991, IEC 801-2: 1991, IEC 801-3: 1984,

IEC 801-4: 1988, EN 61010-1: 1993, EN 60825: 1992

EU Notified Body: Not Applicable Date

Approved by: Date

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ISO 9001/EN ISO 9001:1987
certified by KEMA

269-086300

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Troubleshooting Applications Problems



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

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

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

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 fringes or channeling.	Your sample has parallel, highly reflective sides that cause the infrared beam to bounce within the sample when the sample is placed perpendicular to the infrared beam.	Create a new film using a matte press. Try roughening the film surface slightly with silicon carbide paper or another suitable abrasive. Rotate the sample so that the infrared beam passes through the sample at Brewster's angle. This method should not be used if you are performing a quantitative analysis of the sample.

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Problem	Possible Cause	Solution
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.	If you have an optional purge kit, make sure you are using dried air or nitrogen and that the purge flow rate is set to 15 scfh. Allow the system 3 to 5 minutes to reestablish purge before collecting a spectrum.
	The spectrometer is not purged at all.	If you do not have a purge sytem and the carbon dioxide peaks interfere with your data, you may want to install a purge gas source and optional purge kit. Contact Nicolet for details.
	The spectrometer is purged but your air drier does not remove carbon dioxide.	Replace the air drier with a model that removes carbon dioxide. Contact Nicolet for details.
There are no peaks in a spectrum.	There is no sample in the path of the infrared beam.	Check the sample compartment or accessory to make sure the sample is properly positioned in the beam path.
	The sample cup in the slide of a diffuse reflection accessory is not in place or is tilted.	Make sure the cup is properly positioned in the accessory.
	The infrared microscope is in its viewing mode.	Put the microscope in infrared mode and collect the spectrum again.
	The sample film in an attenuated total reflection (ATR) experiment is being held against the ATR crystal with uneven pressure or has poor contact with the crystal.	Make sure the sample is held evenly and has good contact with the crystal.

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Problem	Possible Cause	Solution
A spectrum contains water peaks that interfere with your data.	The desiccant has expired.	Check the desiccant and replace it if necessary.
	The spectrometer is not adequately purged.	Make sure you are using dried air or nitrogen purge gas and that the purge flow rate is set to15 scfh. Allow the system 3 to 5 minutes to reestablish purge before collecting a spectrum.
A spectrum contains derivative-shaped peaks.	A sample in a diffuse reflection experiment also has a specular reflection component.	Correct the spectrum by using Other Corrections in the Process menu. (Select Kramers-Kronig.)
	The infrared beam was reflected from (instead of penetrating) a flat, shiny sample measured using a specular reflection accessory.	Try using a less reflective sample.
The baseline of a spectrum is not flat.	A KBr pellet was made with coarsely ground KBr powder, or the KBr pellet was improperly pressed.	Be sure to press the pellet properly.
	The background spectrum for a cast film was collected with an empty sample holder.	Remove the sample holder and collect the background again.
	The spectrometer is not properly aligned, causing a sloped baseline.	Use the Align button on the Diagnostic tab in the Experiment Setup dialog box to align the spectrometer.
	The spectrometer has not reached thermal equilibrium.	For best results allow the spectrometer at least 1 hour to stabilize after turning it on.
	The spectrometer is not properly purged.	Check the system to make sure that the correct purge gas is being used and that the flow rate is set to 15 scfh.

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Problem	Possible Cause	Solution
A spectrum is too noisy.	There were too few scans.	Increase the number of scans on the Collect tab in the Experiment Setup dialog box.
	The resolution was too high.	Reduce the resolution on the Collect tab in the Experiment Setup dialog box.
	The purge gas flow rate or pressure is too high.	Check the pressure regulator; it should be set between 10 and 20 psi. Check the flowmeter; it should be set to 15 scfh.
	The moving mirror velocity is set too high for the detector.	For DTGS detectors, reduce the Velocity parameter setting on the Bench tab in the Experiment Setup dialog box to 0.63 or less.
	If this an ATR experiment, the sample is not in good contact with the ATR crystal.	Reapply the sample to obtain more consistent contact between the sample and ATR crystal.

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