



# OMNIC User's Guide

Version 8.0

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# Introduction

Thermo Scientific OMNIC™ software is an advanced software package for FT-IR spectroscopy that lets you perform a wide range of tasks, from collecting infrared spectra to performing quantitative analysis. The commands needed to collect and process spectra are conveniently arranged in menus and can also be entered from the keyboard using shortcut keys.

OMNIC lets you continuously monitor system operation and informs you if a problem is found and explains how to correct it.

Provided with your software are some example experiment files, which contain parameter settings appropriate for different applications and OMNIC tutorials. By selecting one of these experiments (or other experiment you have saved) from the Experiment drop-down list box near the top of the OMNIC window, you can set the spectrometer parameters, library setup options and QCheck comparison settings for your application or a tutorial in one step. (Only previously opened experiments are available in the Experiment drop-down list box. To use another experiment, click the Open button in the Experiment Setup dialog box available through Experiment Setup in the Collect menu. The experiment files are in the My Documents\OMNIC\PARAM directory.)

When you install a Smart Accessory™, the appropriate experiment is automatically selected for you (or a list of appropriate experiments is made available for your selection), and you can begin collecting spectra with the accessory.

When you install a Smart Accessory, the appropriate experiment is automatically selected for you (or a list of appropriate experiments is made available for your selection), and you can begin collecting spectra with the accessory. If Hide All OMNIC Menus is turned on (available through Edit Toolbar in the Edit menu), you must use the Smart Accessory, if any, that is required for the current experiment. If you install a different Smart Accessory, a prompt asks you to replace it.

Your software also includes some example spectral libraries. These are subsets of libraries you can purchase from us. When you view the list of available libraries on the Search Libraries tab of the Library Setup dialog box (available through the Analyze menu), you can identify these libraries by the words “Sample Library” or “Example Library” in the title. You can use these libraries to learn how to set up and perform a library search. For more information about these libraries, see “Example libraries” in the “Analyze” chapter. For information on using Library Setup, see “Setting up a spectral search or QC comparison” in the “Analyze” chapter.

**Note** The Library Converter program lets you various types of spectral libraries to OMNIC format. After a library is converted, you can use it in library searches and QC comparisons within OMNIC. To start the program, click the Start button on the Windows taskbar, point to All Programs, point to the Thermo Scientific OMNIC folder, and click the Library Converter program. ▲

To learn how to use OMNIC or your spectrometer, use the tutorials available in the Help menu. Your system manual contains additional information about using the spectrometer.

**Using OMNIC DS** If you have the DS option, the Security Administration software controls access to OMNIC features. To learn about this software, start by reading “Data security” later in this chapter. If you do not have the DS option, please disregard the information that pertains to these features. ▲

**How to use this manual** This manual describes every feature in the OMNIC application program. The first chapter, “Introduction,” tells you how to get started and how to use the on-line documentation. The second chapter, “About the Display,” explains how spectra are displayed and how you can manipulate data on the screen. The rest of the chapters are organized just like the software; each menu name in the menu bar across the top of the OMNIC window is also the name of a chapter in the manual. The commands contained in the menus are discussed in the same order as they appear in the menus.

The information about a command can include the following:

- What the command does and when to use it.
- How to use the command.
- Tips for using the command.

At the end of the manual is an index that will help you locate information about specific software features.

Many of the spectra used to create the illustrations in this manual are included with the OMNIC software. You may wish to use these example spectra as you learn about the software. The spectra are contained in spectral data files in the Spectra directory within the OMNIC directory.

## Conventions used in this manual

The following conventions are used in this manual to draw your attention to important information.

**Note** Notes contain helpful supplementary information. ▲

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

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

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

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

Any text that you are required to type at the command prompt is underlined in this manual. The Enter key is shown as <Enter>. Here is an example:

```
C: \>WIN OMNIC <Enter>
```

## Starting OMNIC

Follow the steps below to start OMNIC. For information on other methods of starting applications and more detailed instructions on using Windows features, see your Windows documentation.

After you start OMNIC, the OMNIC window appears. The “About the Display” chapter provides complete information on the features contained in the window.

**1. Click the Start button.**

**2. Point to All Programs.**

**3. Point to the Thermo Scientific OMNIC folder.**

**4. Click the OMNIC program.**

- If you have the DS option, you are asked to enter a password. Type the password for the user currently logged into Windows and then choose OK.
- If you do not the DS option but the log-in feature is turned on, you are asked to enter a user name. You may also be asked to enter a password. Type a user name (normally your name) and password, if required, in the appropriate text box and then choose OK.

If you entered a name that is not recognized by OMNIC's log-in feature, a message informs you. Choose OK and then enter a valid name.

If the configuration file associated with the entered user name has a password, a prompt asks for the password. Type the correct password in the text box and choose OK. (If you fail to enter the correct password after three attempts, OMNIC starts but only the Log In and Exit commands in the File menu are available.)

**Note** The Log In command is never available if the system includes the DS option. ▲

See “Turning OMNIC log-in on or off” and “Logging into OMNIC” in the “File” chapter for details on the log-in feature.



## Software security

OMNIC allows you and other users to customize menus, create toolbars and set software options that fit the way each person prefers to use the software. You can save your own configurations in configuration files and open them later to reset the software. To prevent other users from altering configurations you have designed and saved, OMNIC lets you protect each of your configuration files with a password that must be entered before a user can open the file. You specify the password for a configuration file when you save the file.

**Note** If you have the DS option, the Security Administration software is used. Skip the rest of this section and read the “Data security” section. ▲

When you installed the software, you specified whether to prompt a user to log in when starting OMNIC. If this feature is on, OMNIC loads the configuration associated with the name the user entered. To turn this feature on or off after installing the software, use Enable OMNIC Log-In in the File menu. See “Turning OMNIC log-in on or off” in the “File” chapter for details.

### A note for system managers

You can set the system so that other users must log in and cannot turn off the log-in feature. This lets you control who uses the software and which configurations are used. See “How to set up a controlled system” for details. ▲

If you start OMNIC with the log-in feature turned off, the software loads the default configuration file. If the file has a password, a prompt asks for the password. If you enter the correct password, the OMNIC features contained in the configuration become available for use. If you do not enter the correct password (you are allowed three attempts), only the Open Configuration and Exit commands in the File menu become available. Open Configuration lets you use a different configuration file (see “Opening a configuration” in the “File” chapter for details). You can then begin working with the software.

**Note** You can specify which configuration file is loaded when OMNIC starts by using Save Configuration As in the File menu. See “Saving a configuration” in the “File” chapter for details. ▲

When you enter the correct password, it becomes the current password. If you then open or save a configuration file which uses that password, you are not asked to enter it. If you will be away from the computer for long, exit OMNIC to prevent other users from being able to change and save configuration files without entering the password.

**Note** If you accidentally delete all the configuration files from the hard disk, reinstall OMNIC to establish a default configuration file. ▲

After you install OMNIC, the initial configuration (DEFAULT.CON located in the Param directory within the OMNIC directory) does not have a password. To give it a password, use the Password button in the Save Configuration As dialog box.

If you no longer want a configuration file to have a password, use Windows file management features to overwrite the file with another configuration file that does not have a password. (You cannot use the Save Configuration As command for this, as it will not remove a password; it overwrites only the configuration information.) You can also delete a configuration file by using Delete Files in the File menu. *Be careful not to delete all of your configuration files*; OMNIC requires a configuration file in order to start. See your Windows documentation for more information.

**Notice** Whenever you assign a password to a configuration, *be sure to write down the password and keep it in a secure location*. If you forget the password and do not have it written down, you will not be able to use that configuration. ▲

## Data security

If you have the DS option, the Security Administration software is used to set and enforce security policies for OMNIC. This includes the following:

- Controlling access to OMNIC menu commands.
- Establishing system policies affecting such things as preventing the overwriting of files and requiring electronic signatures.
- Specifying the meanings that will be available for electronic signatures supplied by users.

See the *Security Administration User's Guide* and the manual titled *Setting Up OMNIC DS* for complete information about using the data security features. You can use these features to help you comply with the regulations contained in 21 CFR Part 11, the United States Food and Drug Administration document for electronic records and electronic signatures. For more information about this document, see the document titled *OMNIC Software: 21 CFR Part 11 Compliance*.

In addition to the data security features provided in Security Administration, OMNIC has menu commands that let you digitally sign a file or verify that a file has been digitally signed. See “Signing a file” and “Verifying a digital signature” in the “File” chapter.

**Note** For maximum protection of your configurations, experiments, quant methods and other important files, we recommend placing them in directories for which users other than the administrator do not have write and delete permissions. This will prevent these files from being overwritten or deleted outside OMNIC by unauthorized users. ▲

## Digital signatures

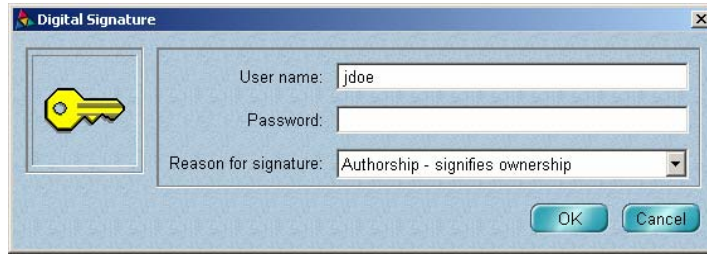
This section explains how to provide a digital signature when you are prompted for one and how to sign a file when you save it. It also describes the digital signature information that appears in a spectral window when you open a spectrum. This section applies only to systems that include the DS option.

### Providing a digital signature

You may be prompted during a procedure to provide a digital signature. The visible portion of a digital signature consists of a user name, a date and a stated reason for signing. A digital signature also contains encrypted information that lets you detect whether the file has changed since it was signed.

**Note** You can sign a file only after it has been saved on a disk. You cannot sign a spectrum, report, etc. while it is in memory but not yet saved on a disk. ▲

Here is an example of such a prompt:



Follow these steps to respond to the prompt:

**1. Verify that the correct user name appears in the User Name text box.**

Only the currently logged-in user may sign a file.

**2. Type your password in the Password text box.**

**3. Select the appropriate signature meaning from the Reason For Signature drop-down list box.**

The listed meanings may vary depending on the security policies of your system and may include Authorship, Approval, Review, Revision or others. These meanings can be used for meeting requirements described in *OMNIC Software: 21 CFR Part 11 Compliance*.

You may also be able to type a custom signature meaning in the Reason For Signature box.

**4. Choose OK.**

A message states that the file was successfully signed.

**5. Choose OK.**

**Signing a file when you save it**

When you save a spectrum, experiment or configuration, you can sign the file by turning on the Use Digital Signature check box in the dialog box that appears.

When you click the Save button in the dialog box, you are prompted for a digital signature. Follow the steps in the preceding section to provide the signature.

**Note**

Signing a file in this way has the same effect as using the Sign File command in the File menu. ▲

**Digital signature information in a spectral window**

When you open a stored spectrum to view it in a spectral window, digital signature information appears in the upper-left corner of the pane:

- If the file has not been signed, “Signature: Not Signed” appears.
- If the file has been signed and has not been changed since it was signed, the name of the person who signed it appears, along with the date and time of the signature and the reason for signing; for example, “Signature: Smith, John, 02-21-2001 12:02:37 (GMT-06:00), Authorship.” (The “GMT-06:00” indicates the location relative to Greenwich Mean Time.)
- If the file has been signed and has been changed since it was signed, the following text appears: “Unable to verify digital signature. The data has been changed.”

**Digital signature information in the Collection And Processing Information window**

A spectrum’s signature history appears in the CURRENT DIGITAL SIGNATURE STATUS section of its collection and processing information. You can see this information by clicking the Information button, labeled “i,” to the left of the title box. See “Collection and processing information” in the “About the Display” chapter for more information.

**How to set up a controlled system**

By using the following procedure, you can set up the system so that other users are required to log in when they start OMNIC, and use the software configuration you have specified.

**Note for DS systems** This procedure is not intended for systems that include the DS option. See the manual titled *Security Administration User's Guide* for a procedure for setting up a controlled system with the DS option. ▲

**Note** This procedure is intended for system managers. If the manager has already set up a controlled system, some of the features discussed below may be unavailable in the configuration you are using. ▲

**1. Use Options, Edit Menu and Edit Toolbar in the Edit menu to set up OMNIC the way you want other users to use it.**

See “Customizing OMNIC by setting options,” “Customizing a menu” and “Customizing a toolbar” in the “Edit” chapter for details.

If you already have a configuration saved with the desired settings, skip to step 5.

To have a secure system whose configuration cannot be altered by an unauthorized user, we recommend using Edit Menu to disable or hide the following commands:

- Enable OMNIC Log-In in the File menu
- Add User Name in the File menu
- Open Configuration in the File menu
- Save Configuration As in the File menu
- Edit Menu in the Edit menu
- Edit Toolbar in the Edit menu

**2. Save the current configuration using the name STUDENT.CON or some other appropriate name.**

**3. Open the default configuration (DEFAULT.CON) to restore full access to the software features.**

**4. Save the default configuration (using the name DEFAULT.CON) and assign a password to it.**

This will prevent unauthorized users from opening the configuration to gain full access to the software features.

- 5. If the log-in feature is not already on, turn it on by choosing Enable OMNIC Log-In from the File menu.**

A check mark appears next to the command name when the feature is on. See “Turning OMNIC log-in on or off” in the “File” chapter.

- 6. Use Add User Name in the File menu to add the name of a user who will be using the limited configuration you saved in step 2.**

When the Select Configuration File dialog box appears, select that configuration (STUDENT.CON in this example). See “Adding a user name” in the “File” chapter for details.

- 7. Repeat step 6 for each additional user who will be using the limited configuration.**

- 8. Use Add User Name in the File menu to add the name of the authorized manager of the system.**

When the Select Configuration File dialog box appears, select the appropriate configuration (DEFAULT.CON in this example).

- 9. Exit OMNIC, restart OMNIC and then use Log In in the File menu to test the newly added user names.**

The limited configuration should be opened when you log in as one of the “students,” and the configuration allowing greater access to features should be opened when you log in as the manager. See “Logging into OMNIC” in the “File” chapter if you need more information.

## On-line Help

OMNIC includes several kinds of on-line documentation to give you easy access to useful information. There on-line tutorials, a wizard and a complete Help system.

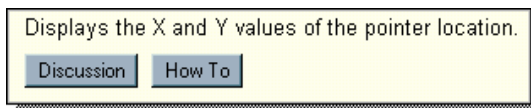
You can start a **tutorial** by choosing it from the Help menu or by clicking a button or text that shows the name of the tutorial within a Help topic.

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

The OMNIC on-line **Help system** lets you quickly find answers to your questions about using the software. It contains Discussion topics that describe how features work and when you should use them, and How To topics that explain step by step how to use the features. You can click buttons or underlined text to move from one topic to another. The Help system also offers a table of contents, a complete index, and a way to search for text in any topic. All these features are explained below.

There are several ways to enter the Help system.

- You can see information about many features in OMNIC (such as a menu command, a parameter in a dialog box, etc.) by clicking the feature using the right mouse button. (If the active dialog box or window includes a question mark button near the upper-right corner, you may need to first click that button and then click the feature of interest using the left mouse button.) A brief description appears, and in most cases one or more buttons you can click to display more details. Here is an example:



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

- You can press the F1 function key at any time to see a discussion topic for the currently displayed or selected feature, dialog box or window.
- If a dialog box or window contains a Help button, click it to see information about the dialog box or window (or the command that displayed it).
- To see the Contents of the OMNIC Help system, choose OMNIC Help Topics from the Help menu.



If you have not used Windows Help before, see your Windows documentation for more information. You can also choose Using Help from the Help menu to see information on using the Help features.

**Tutorials** OMNIC includes on-line tutorials to help you learn how to perform a variety of tasks with your spectrometer. To use a tutorial, choose it from the Help menu. (Some of the tutorials “pop up” when you point to items in the menu that have an arrow symbol to the right of the item name.)

**Note** Some tutorials are available only for particular spectrometer models. ▲

Before you use a tutorial, open the provided experiment that contains the appropriate parameter settings for that tutorial. If you have changed the parameter settings in the experiment, you can quickly restore them to their default settings before using it. See “Restoring the default settings” in the “Collect” chapter for details.

For descriptions of the available tutorials, choose OMNIC Help Topics from the Help menu, find “tutorials” on the Index tab and go to the “Tutorials” topic.

## **Questions or concerns**

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



# About the Display

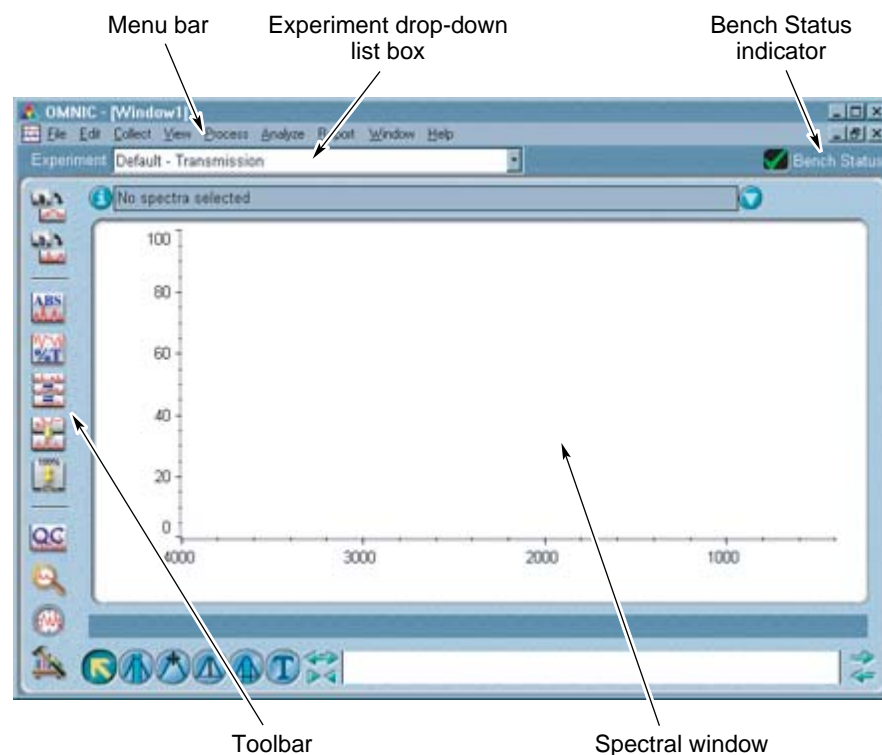
This chapter describes the unique display features of your OMNIC software. You should understand how to use these features before going on to collect or process data.

You can customize the way OMNIC displays spectra by setting options using the Options command in the Edit menu. See “Customizing OMNIC by setting options” in the “Edit” chapter for details.

## The OMNIC window

While you are using OMNIC, the OMNIC window is displayed on the screen.

Within this window one or more spectral windows can be displayed, each of which can contain spectra and other forms of spectral data.



The menu bar at the top of the OMNIC window contains the menu names. The menus are arranged in an order that is convenient for collecting and processing data. Within each menu, the commands are grouped according to their related functions.

You choose commands in OMNIC just as in other Windows applications: by using the mouse or by typing key combinations on the keyboard. If a command displays a dialog box or task window, it appears within the OMNIC window.

## Monitoring the spectrometer status

If you have a Nicolet™ iS™ 10, Nicolet 380, Nicolet 4700, Nicolet 5700, Nicolet 6700, Nicolet 8700, Nicolet Nexus™, Magna-IR™, Nicolet Protégé™ or Nicolet Avatar™ spectrometer and Survey Bench And Smart Accessory is turned on in the Collect options, OMNIC continuously monitors the spectrometer operation and informs you if a problem is found and explains how to correct it. The System Status indicator below the menu bar shows the status of the spectrometer operation.



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



If the indicator is a yellow shield containing an exclamation mark, either of two conditions exists: A cooled detector has become warm, or data cannot be collected on a Nicolet Avatar spectrometer because the printer port is being used to print information. A message explains the problem and lets you access information on correcting it.



If the indicator is a red X, the spectrometer has failed a diagnostic test and requires corrective action, or the computer cannot communicate with the spectrometer. A message explains the problem and lets you access information on correcting it.

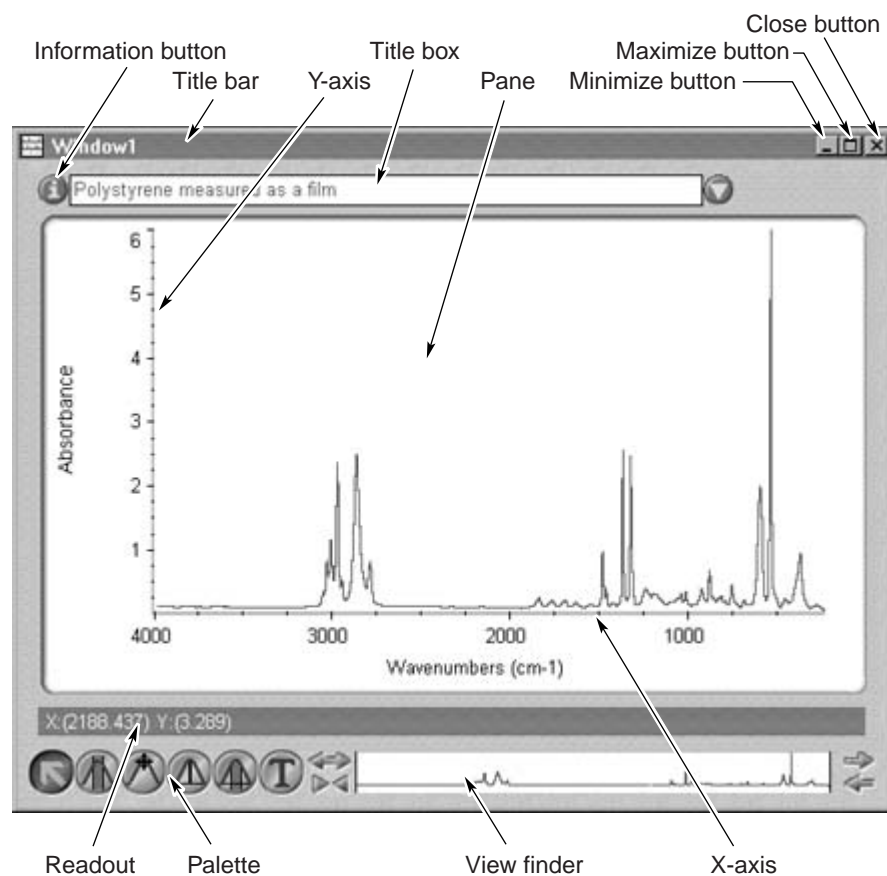
See “Surveying the spectrometer and Smart Accessory” in the “Edit” chapter for details on turning this option on or off.

## Spectral windows

Spectral windows let you view several kinds of spectral data, such as spectra you have collected or processed or library spectra found in a spectral search.

The following illustration shows a spectral window containing a single spectrum and identifies the main parts of the window.

Many spectral windows can be displayed on the screen at once. The exact number depends on the amount of memory in your computer.



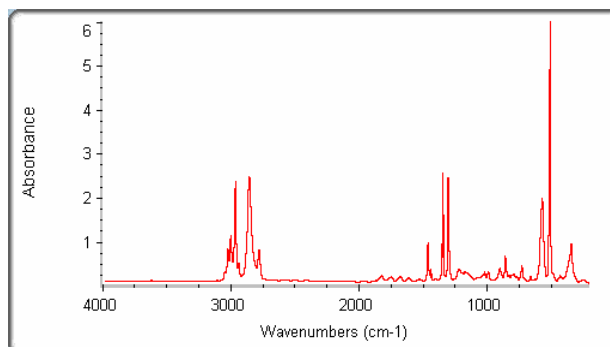
Depending on the software option settings, a new spectral window may be created when you perform operations such as retrieving a spectrum from a disk or adding a spectrum you just collected to a spectral window. You can also create a new spectral window by choosing New Window from the Window menu (see “Creating a new spectral window” in the “Window” chapter for details).

If you make any changes to a spectrum in a spectral window and then close the window, a message may appear asking whether to save the changes. (The message appears only if Prompt Before Closing Spectral Windows is turned on in the Process options. See “Saving spectra before closing spectral windows” in the “Edit” chapter for more information.) To save your changes, choose Yes. To close the window without saving the changes, choose No. To leave the window open, choose Cancel.

The following sections explain the features of spectral windows.

## Panes

A pane is an area of the spectral window used to display a spectrum along with associated information and software features. Here is an example of a spectrum displayed in a pane:



A spectral window can contain one or several panes, as specified by Display Setup and the Window options (available through Options in the Edit menu). You can display spectra in Overlaid or stacked panes, depending on how you want to view the data. See “Setting the display parameters” in the “View” chapter and “Window options” in the “Edit” chapter for information on setting the number of panes.

## The active spectral window

Only one spectral window can be active (selected) at a time. The active spectral window is the one affected by operations you perform. To make a spectral window active, click anywhere within it or choose its title from the Window menu. The title bar of the active spectral window is displayed in the color you specify using Control Panel. (See your Windows documentation for information on using Control Panel.)

## Display colors

You can display several spectra in a spectral window at one time. To help differentiate the spectra, they are displayed in different colors. Eight colors are available and are assigned as spectra are added.

When a spectrum is selected, it is displayed in the color specified for selected spectra. A selected spectrum is a spectrum on which you can perform operations. See “Selection tool” for information on selecting spectra.

To change the color of the spectra in a spectral window, use Display Setup in the View menu or the Colors button in the View options. See “Setting the display parameters” in the “View” chapter and “Specifying colors for spectra and other features” in the “Edit” chapter for more information.

## Resizing a spectral window

To resize a spectral window, drag one of its borders or corners or click the Maximize button or Restore button. (You can also click the Minimize button to shrink the window.) The window's title box, palette and view finder are scaled proportionately. The panes, spectra and axes are also scaled to fit the window.

**Note** When a spectral window is maximized, it shares a title bar with the OMNIC window. ▲

## Axes

Along the bottom and left side of a pane (or panes) in a spectral window are the axes. The scale and display limits of the X-axis depend on the spectral region you are displaying. If you display a different region by using the view finder or selection tool, the X-axis is automatically adjusted for the new region. See “View finder” and “Selection tool” for an explanation of how to display different regions.

For normal FT-IR applications, the most commonly used X-axis units are the wavenumber ( $\text{cm}^{-1}$ ) and the micrometer ( $\mu\text{m}$ ). You can specify the unit by using Display Setup in the View menu. See “Selecting an X-axis format” in the “View” chapter for illustrations of X-axes with these and other units.

**Note** The scale of the X-axis is usually uniform across the spectrum. Sometimes, however, it is easier to see important peaks if a different X-axis scale is used for different regions. Use X-Axis Format in the Display Setup dialog box to split the X-axis into two or three sections, each with a different scale. ▲

The unit used for the Y-axis depends on the final format used when the spectrum was collected and whether you have converted the spectrum to another format. You can set the initial Y-axis unit for collected spectra by using Experiment Setup in the Collect menu (see “Selecting the final format” in the “Collect” chapter for details). The first three commands in the Process menu let you convert the spectra to absorbance, % transmittance, Kubelka-Munk, photoacoustic, % reflectance or  $\log(1/R)$  units. The “Process” chapter explains how to use these commands.

During data collection, the Y-axis unit is the volt, a measure of the interferogram signal. When the interferograms are transformed into a single-beam spectrum, the Y-axis unit used expresses the intensity of the infrared energy versus frequency.

Processing interferogram or single-beam data to any other Y-axis units requires a background spectrum. A background spectrum contains information about the instrument and the atmosphere inside the spectrometer or sampling accessory. To remove this information from a sample spectrum, the single-beam sample spectrum is divided by, or ratioed against, the single-beam background spectrum. The resulting spectrum is in % transmittance (or other specified final format) and can be displayed in a spectral window. You can use commands in the Process menu to convert this spectrum to the other Y-axis units, depending on how the sample was measured and the display format you want to use.

The “Scale” commands, Display Limits and Roll/Zoom Window in the View menu let you adjust the Y-axis scale. See the “View” chapter for complete information.

**Note** To turn the display of the axes on or off in existing spectral windows, use Display Setup in the View menu. To turn the display of the axes on or off when a new spectral window is created, use the Window options (available through Options in the Edit menu). See “Setting the display parameters” in the “View” chapter or “View options” in the “Edit” chapter for details. ▲

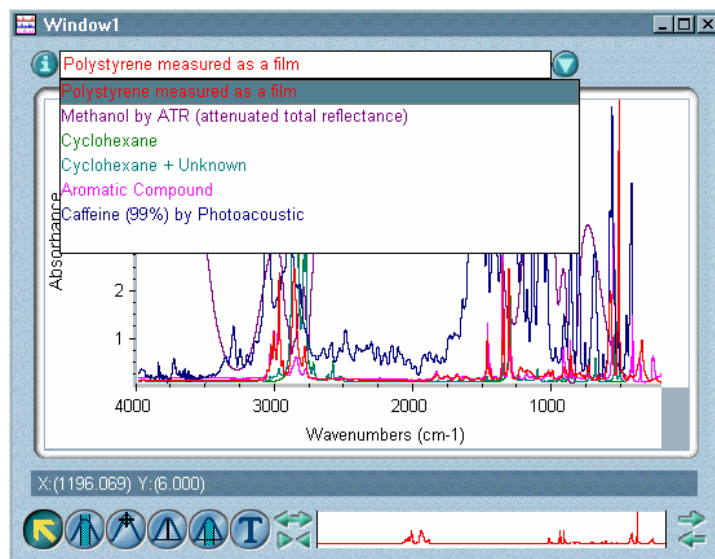
**Title box** The title box near the top of a spectral window shows the title of the spectrum that was last selected or that is currently selected. A selected spectrum is a spectrum on which you can perform operations. If two spectra are selected, the title in the title box changes to “Two spectra selected.” If more than two spectra are selected, “Multiple spectra selected” appears in the title box.

**Displaying a list of spectrum titles** To display a list of spectrum titles, click the arrow to the right of the title box, or click inside the title box and then press the down arrow key on the keyboard (if the title box is already active, just press the down arrow key). A list of the titles of all the spectra in the window appears (see the following example).



If there are too many titles in the list to be displayed at once, a scroll bar lets you scroll them into view.

The title of each selected spectrum is highlighted in the list of titles.



### Selecting listed spectra

There are several ways to select spectra using the title box when the list of spectra is displayed. The following are the two most commonly used methods:

- You can select a spectrum by clicking its title in the list.
- You can select more than one spectrum by holding down the Control key and clicking the desired spectrum titles in the list.

You can also use these methods:

- If one spectrum is selected, you can select a sequence of spectra by holding down the Shift key and clicking the title of the last spectrum in the sequence.
- You can select a sequence of spectra by pointing to the title of a spectrum, pressing and holding down the mouse button, dragging up or down to select additional spectra and then releasing the mouse button.
- You can use the up or down arrow keys to highlight the title of the spectrum you want to select. At least one spectrum must be selected to use this method.

**Note** If at least one spectrum is selected, you can use the arrow keys to select a different spectrum even when the list of spectrum titles is not displayed. ▲

### **Deselecting a listed spectrum**

To deselect a listed spectrum, hold down the Control key and click the title of the selected spectrum in the list of spectra.

### **Removing the list of spectra from the screen**

To remove the list of spectra from the screen, press Tab, click outside the title box, or press Enter. The currently selected spectra remain selected.

### **Selecting a different spectrum using the arrow keys**

If the list of spectra is not displayed but one spectrum is selected, you can select a different spectrum by first selecting the current title in the title box and then pressing the up or down arrow keys. If you press the down arrow key, the next spectrum in the list (if there is one) will be selected and its title will appear in the title box. If you press the up arrow key, the preceding spectrum in the list (if there is one) will be selected and its title will appear in the title box.

#### **Note**

To select the current title in the title box, click it or repeatedly press the Tab key until the title is selected. ▲

### **Changing the title of a spectrum**

Use standard Windows editing techniques to change the title of the spectrum directly in the title box. You can drag to select text in the title and type new text or use Cut, Copy or Paste in the Edit menu to edit the title text. When you are finished editing, click outside the title box or press Enter. To cancel the changes you have made and keep the original title, press Escape. See “Cutting an item,” “Copying an item” and “Pasting an item” in the “Edit” chapter for more information on the commands used for editing text.

We recommend using titles that are specific and include information about how the spectrum was collected or processed.

### **View finder**

The view finder lets you adjust the display of all the spectra in a spectral window or task window to show a larger or smaller spectral region or a different region of the same size. You can also adjust the vertical scale of the selected spectra.

The view finder contains a small image of the entire selected spectrum, regardless of which region of the spectrum is currently displayed. If more than one spectrum is selected in a spectral window, an image of the first spectrum selected appears in the view finder. If no spectrum is selected, the view finder is empty.

If more than one spectrum is displayed in a spectral window, the horizontal range of the view finder encompasses the ranges of all the spectra. The currently displayed spectral region is indicated by the region markers, the blue vertical lines within the view finder.



**Expanding or contracting the display horizontally** – To expand all the spectra horizontally about the center of the pane, click the top half of the view finder’s Horizontal Expand/Contract button. To contract the spectra horizontally about the center, click the bottom half of the button. You can press and hold down the mouse button during these operations to continuously expand or contract the display.

**Note** You can also use the Roll/Zoom window to expand or contract the display. See “Rolling and zooming spectra” in the “View” chapter for details. ▲



**Expanding or contracting the display vertically** – To expand all the selected spectra vertically, click the left half of the view finder’s Vertical Expand/Contract button. To contract the spectra vertically, click the right half of the button. You can press and hold down the mouse button during these operations to continuously expand or contract the display.

**Note** You can also use the Roll/Zoom window to expand or contract the display. See “Rolling and zooming spectra” in the “View” chapter for details. ▲

**Displaying a different spectral region of the same size** – There are three ways to use the view finder to display a different spectral region of the same size:



- To move your view of the spectrum to the right (“roll” to the right), click the right arrow in the top half of the Roll button. To roll to the left, click the left arrow in the bottom half of the button. You can press and hold down the mouse button during these operations to roll continuously to the right or left.
- Point anywhere between the region markers, press and hold down the mouse button, drag the markers to the desired location and release the mouse button.

**Note** You can also use the Roll/Zoom window to roll. ▲

**Note** If you use the Roll button to completely compress a spectrum against one end of the view finder, you must click the bottom half of the Horizontal Expand/Contract button before you can use the Roll button again. ▲

- Click to the left of the left region marker or to the right of the right region marker. Whenever possible, the new displayed region will be centered on the location you clicked. The markers will move so that the clicked location is halfway between the markers.

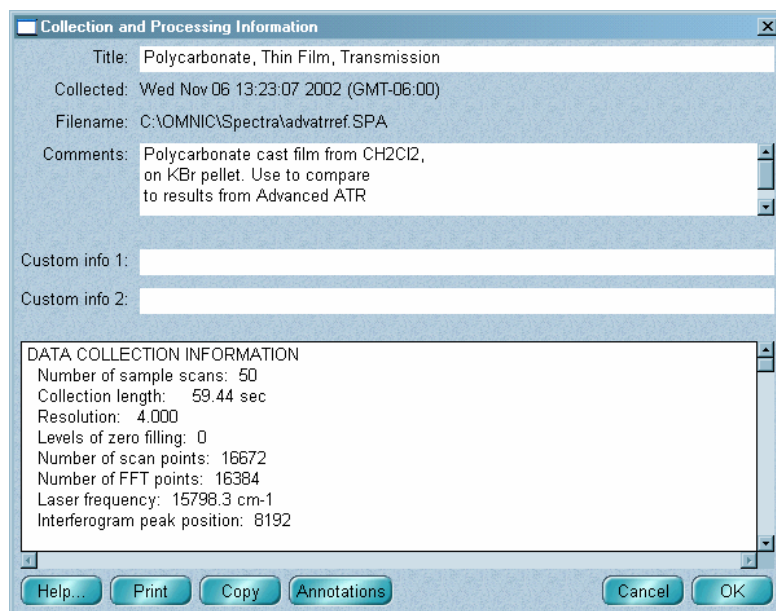
**Changing the display limits by moving the region markers** – Drag a marker left or right to the desired location. The current X values of both markers appear in a box above the view finder while you drag the marker.

**Displaying the entire spectrum** – Double-click between the region markers.

## Collection and processing information

To see information about how the selected spectrum was collected and processed, click the Information button (labeled “i”) to the left of the title box or double-click the spectrum’s title in the title box. To see information about a spectrum that is not selected, first click the arrow to the right of the title box to display the list of spectrum titles and then double-click the title of the spectrum. The Collection And Processing Information window appears:

Scroll bars at the right side and bottom of the window let you see information that doesn’t fit in the window when it is first displayed.



The upper portion of the window includes fields in which you can enter or modify information, such as the spectrum title or comments. See the list of operations below for instructions.

The lower portion of the window contains information about how the spectrum was collected and processed. This information is generated automatically by OMNIC and cannot be modified. You can display some of this information in the spectral window. See “Setting the display parameters” in the “View” chapter for details.

Information about how the spectrum has been modified appears in the “Data Processing History” section. This information can be used as part of an audit trail for the spectrum. If you have OMNIC DS, the user name and digital signature history appear in this section. The current digital signature always appears in the spectral window.

You can edit text, enter custom information to be printed later, copy information to the Windows Clipboard, view and copy information about peak annotations, and print information. The next sections explain these operations.

When you are finished using the window, close it by choosing OK. If you don't want to save the changes you made to the information, choose Cancel.

### **Editing information**

To edit the collection and processing information, click inside the Title, Comments, Custom Info 1 or Custom Info 2 text box. This places an insertion point at the location you clicked. You can delete text using the Backspace key and type new text. If you edit the comments, press Enter wherever you want a line to end when the comments are displayed in a pane (see the following Note). The text after that point will begin at the start of the next line.

### **Note**

The comments for spectra are displayed in a spectral window's panes if the Sampling Information check box and Comments check box are both turned on in the Display Setup dialog box. See “Setting the display parameters” in the “View” chapter for details. ▲

**Entering custom information to be printed later**

If you plan to print the spectrum, you can specify one or two pieces of information to be printed with it by typing the information in the Custom Info 1 and Custom Info 2 text boxes. Show Info Box must be turned on in the Print options (available through Options in the Edit menu) for this information to be printed. See “Printing an information box with spectra” in the “Edit” chapter for more information.

**Note**

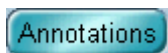
When you add a spectrum to a spectral window using the Add To Window button in Library Manager, an identifying number is placed in the Custom Info 1 text box. See “Placing a library spectrum into a spectral window” in the “Analyze” chapter for more information. ▲

**Copying information to the Clipboard**



Click the Copy button to copy all the information contained in the Collection And Processing Information window to the Windows Clipboard. You can then paste the information into a document using another application that uses the Clipboard.

**Viewing and copying information about peak annotations**



Use the Annotations button to view and copy information about peak annotations. Follow these steps:

1. **Click the Annotations button in the Collection and Processing Information window.**

The Annotation Information window appears. Here is an example:

Annotation Information					
X Position	Text	Baseline Start	Baseline End	Area Start	Area End
1492.63	Corrected Area=15.42	1698.98	1419.35	1498.42	1484.92
1600.63	Area=10.83			1610.44	1589.24
2932.25	Corrected Ht=1.69	3328.53	2674.78		
3026.40	Height=2.33				

The window lists information about peak annotations created with the Annotate button, the annotation tool and Find Peaks in the Analyze menu. (The Annotate button appears when you use the region tool, spectral cursor tool, peak height tool or peak area tool.) For each annotation the window shows the X value of the annotated peak, the annotation text (such as the measured peak height or area), and the starting and ending X values of the baseline and measured area, if appropriate.

2. **If desired, change the information in the Text column by double-clicking a cell you want to change and then editing the text.**

Only the information in the Text column can be changed.

3. **If you want to copy the listed information to the Windows Clipboard, click the Copy button.**

You will be able to paste the information into a document using another Windows application that uses the Clipboard.

4. **When you are finished, choose OK.**



### Printing information














Click the Print button to print the contents of the Collection And Processing Information window on the default system printer.

### Palette

The palette of a spectral window contains six tools that allow you to perform the operations described in the table below. The palette is located in the lower-left corner of every spectral window and the windows that appear during data collection. The names and appearance of the palette tools indicate their functions.

To do this...	Use this tool...
Select items on the screen.	 selection tool
Expand or contract a spectrum.	 selection tool

To do this...	Use this tool...
Move an overlaid spectrum up or down within its pane.	 selection tool
Move a stacked spectrum into another pane.	 selection tool
Drag a spectrum into another spectral window.	 selection tool
Select annotations to be deleted.	 selection tool
Select a region of a spectrum or measure the uncorrected area of a region.	 region tool
Display X and Y values of points.	 spectral cursor tool
Measure the height of a peak.	 peak height tool
Measure the area under a peak.	 peak area tool
Label spectral features.	 annotation tool
Add text to be displayed or printed.	 annotation tool
Move sampling information or annotations.	 annotation tool

Only one tool can be used at a time. To use a tool, select it by moving the mouse pointer over the tool and clicking. The selected tool is highlighted on the screen. A tool remains selected until you select another tool.

If you have selected any tool except the selection tool, when you move the pointer into a pane, a symbol representing the tool appears next to the pointer arrow to help you identify the tool being used.

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.

To display the name of a tool on the palette, point to the tool and wait a moment.



To display more information about the palette, click it using the right mouse button.

The use of each palette tool is explained in the following sections.

### Selection tool

When selected, the selection tool lets you perform these operations:



- Select a spectrum.
- Select an additional spectrum.
- Deselect a spectrum.
- Expand and area of a spectrum.
- Reduce the size of a spectrum.
- Move a spectrum up or down.
- Move a stacked spectrum into another pane.
- Drag spectra into another spectral window.
- Selecting annotations.

Each of these operations is explained later in this section.

As you move the pointer across a pane, the X and Y values of the current pointer location are shown in the readout above the palette. This feature can help you position the pointer when you use the selection tool to perform some of the operations listed above.

The following summary explains the uses of the selection tool. In each use described, the tool has already been selected.

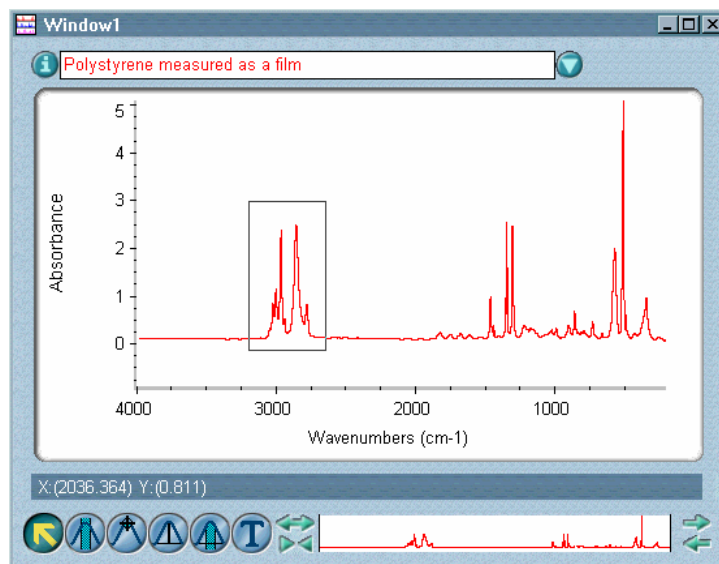
**Selecting a spectrum** – Click the spectrum. The spectrum becomes selected, and any other spectra that were selected are no longer selected (unless the Control key was held down to select multiple spectra). When a spectrum is selected, it is displayed in the color specified for selected spectra, and its title appears in the title box. See “Title box” for more information.

**Selecting additional spectra** – Hold down the Control key, click each spectrum you want to select and then release the Control key. The spectra you click become selected, and any other spectra that were selected remain selected. You can select any number of spectra in a spectral window can at the same time. When multiple spectra are selected, all of them are affected by an operation you perform.

**Note** You can select all the displayed spectra in a spectral window by choosing Select All from the Edit menu. See “Selecting all the spectra in a spectral window” in the “Edit” chapter for details. ▲

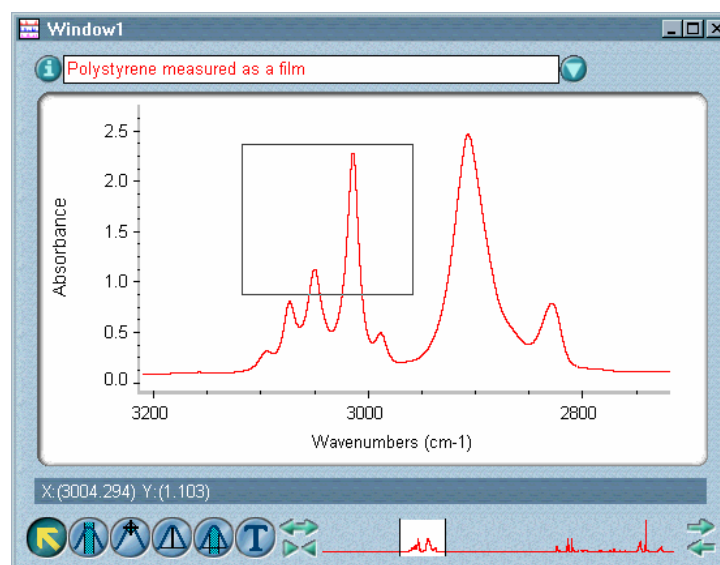
**Deselecting a spectrum** – Hold down the Control key and click the selected spectrum. The spectrum you click is deselected, but all the other selected spectra remain selected. You can deselect all the spectra except one by clicking (without the Control key held down) the spectrum you want to remain selected. The rest of the spectra are deselected.

**Expanding an area of a spectrum** – Draw a box around the area you want to expand. First point to where you want to locate a corner of the box. This point should be at the desired minimum or maximum X value and minimum or maximum Y value. Press and hold down the mouse button, drag the pointer to a location for the opposite corner and then release the mouse button. See the following example.



Next, click inside the box. The area inside the box expands to fill the pane and the box disappears. The new display limits of the axes are those of the box. If you change your mind before clicking inside the box and want to expand a different area, first remove the box from the screen by clicking a location outside the box and then repeat the action described above.

**Reducing the display size of a spectrum** – Draw a box in the pane. To do this, point to where you want to locate a corner of the box, press and hold down the mouse button, drag the pointer to a location for the opposite corner of the box and then release the mouse button. See the example below.



Next, hold down the Shift key and click inside the box. The spectrum is scaled so that the previously displayed portion fits in the area defined by the box. Since the spectrum is reduced in scale, more of it is displayed in the pane (unless it was already fully displayed).

**Moving an overlaid spectrum up or down within its pane** – Drag the spectrum. As you drag it, an image moves up or down on the screen, indicating the new vertical location. When you release the mouse button, the spectrum is displayed with the dragged point at the vertical position of the pointer. The Y-axis changes to reflect the new position. The Y values of points in the spectrum do not change.

This feature is useful when you want to offset spectra in a window to compare them or see them better.

See “Overlaying and stacking spectra” for more information on overlaid spectra.

**Moving a stacked spectrum into another pane** – Drag the spectrum into the desired pane in the same spectral window. The spectrum is moved from its original pane into the new pane. If there already is a spectrum in the new pane, the locations of the two spectra are switched.

If a pane is locked, you must first unlock it (by clicking the box in the upper-right corner of the pane) before you can move a spectrum into it or out of it.

If more than one spectrum is selected when you attempt to move the spectra, only the spectrum that was selected last is moved.

See “Overlaying and stacking spectra” for more information on stacked spectra.

**Dragging spectra into another spectral window** – Follow these steps:

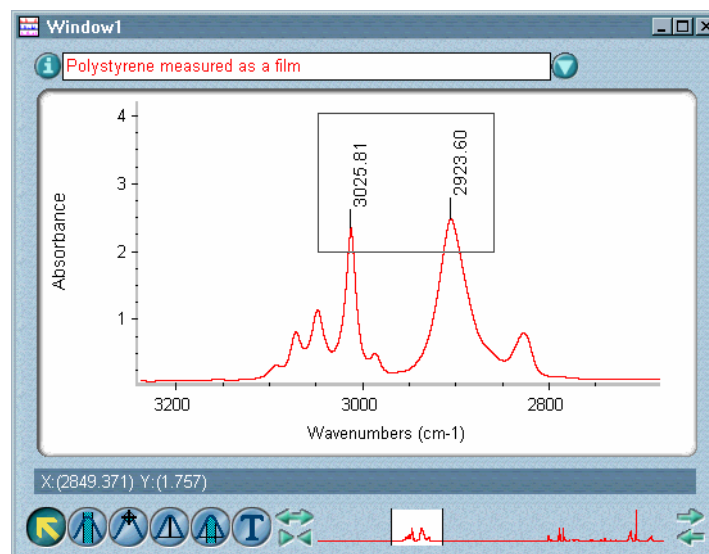
- 1. Arrange the two spectral windows so that both are visible.**
- 2. Select the spectra.**
- 3. Drag the spectra into the second spectral window.**

To do this, point to the spectrum, press and hold down the left mouse button, move the pointer to the second spectral window, and release the mouse button.

As you drag the spectrum, the pointer appears as a small graphical image of a spectrum with a plus (+) sign at the top to indicate where you are moving the spectrum. If you attempt to drag the spectrum to a location where it cannot be placed, the pointer appears as a circle with a line through it. If this image appears, drag the spectrum into a spectral window pane.

When you release the mouse button, a copy of each spectrum appears in the second window. The original spectra remain in the first window.

**Selecting annotations** – Select the spectrum and then draw a box around the annotations (see the example below).



To draw the box, point to where you want to locate a corner of the box, press and hold down the mouse button, drag the pointer to a location for the opposite corner of the box and then release the mouse button. Be sure to enclose all the text of the annotations with the box; otherwise, the text will not be selected. There is no need to enclose the lines that connect the annotations to the spectrum.

After you have selected the annotations, you can delete them by using Delete Annotation in the Edit menu or by holding down the Control key and clicking inside the box. See “Deleting annotation” in the “Edit” chapter for details.

### Region tool



Some OMNIC commands can be used to operate on a region of a spectrum rather than on the entire spectrum. For example, you can use Blank to delete a spectral region that contains unwanted absorptions. To select a spectral region for these commands, use the region tool before choosing the command.

You can also use the tool to measure the uncorrected area under peaks. The uncorrected area is measured from zero absorbance instead of the baseline. (In a transmittance spectrum, the uncorrected area is measured from 100% transmittance.) By using the Annotate button after area measurements, you can annotate peaks with their areas and then print the spectrum with these annotations.

**Note** You can use Options in the Edit menu to specify the text orientation, font and number of decimal places for area annotations. See “View options” in the “Edit” chapter for details. ▲

**Note** You can measure the corrected area under a peaks by using the peak area tool. ▲

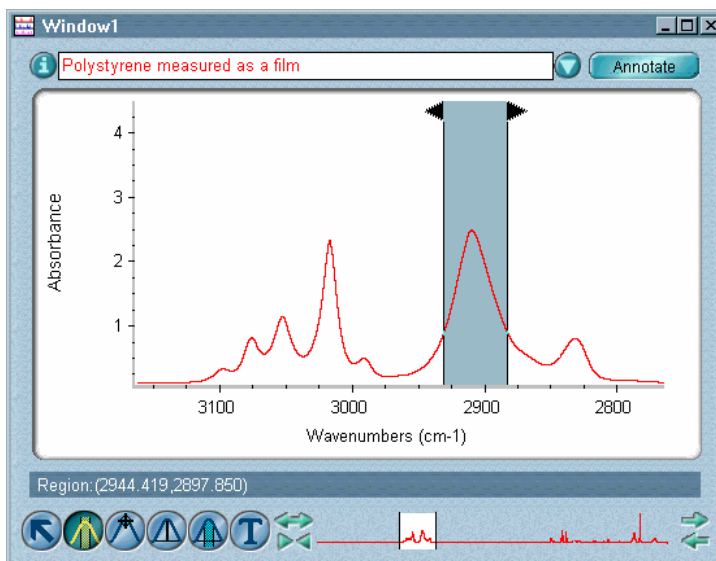
**Selecting a spectral region** – Follow these steps:

- 1. Select the spectrum that contains the region.**
- 2. If necessary use the view finder or selection tool to display the entire region.**
- 3. Select the region tool.**
- 4. Point to where you want the region to start and press and hold down the mouse button.**
- 5. While holding down the mouse button, move the pointer to where you want the region to end. Then release the mouse button.**

As you move the pointer, two vertical lines appear at the limits of the region. The X-axis limits and width of the region are displayed in the readout above the palette.

When you release the mouse button, the region between the vertical lines is shaded to indicate that it is selected (see the following example).

As long as this region remains selected (shaded), it will be used by the next operation you perform that operates on a selected region.



If you open another spectrum or select one by using the up or down arrow keys on the keyboard, the same region will be selected in that spectrum.

At the top of each vertical line is a triangular handle that you can drag to the left or right to change the region limit.

You can use the Annotate button to label the region with its uncorrected area (see the next procedure).

**Measuring the uncorrected area of a peak** – Follow these steps:

- 1. Select the spectral region (peak region) that you want included in the area measurement.**

See the preceding procedure for instructions. When you release the mouse button, the portion of the shaded region that is under the peak is used to calculate the area. You can drag the triangular handles to make the region larger or smaller.

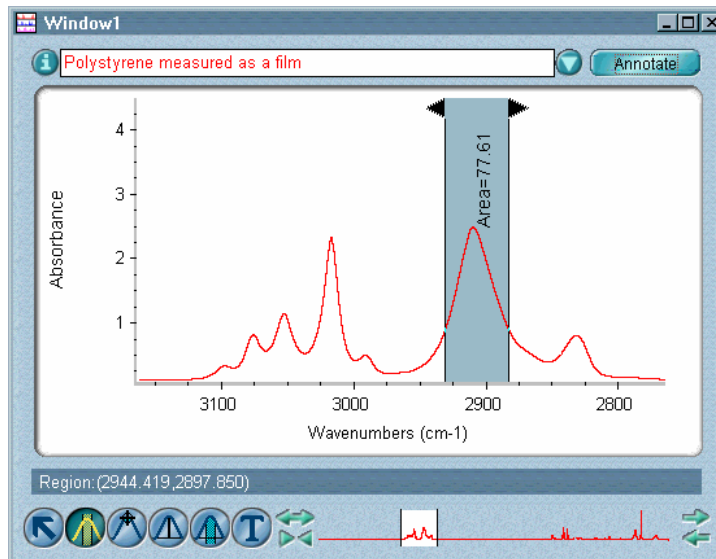
You can start over by selecting a different region before clicking the Annotate button in the next step. (After you click the Annotate button, you will need to delete the annotation if you want to start over.)

**2. Click the Annotate button to the right of the title box.**

**Note** The Annotate button is available only if Annotation is turned on in the Display Setup dialog box. ▲

The uncorrected area measurement appears as an annotation near the peak.

You can position the annotation text by using the annotation tool.



You can measure the area of another peak by repeating steps 1 and 2.

After you click the Annotate button, the annotation remains on the screen when you label another peak or use another tool. The uncorrected peak area is shaded and extends to zero absorbance units (or 100% transmittance). Vertical lines show the frequency limits of the area.

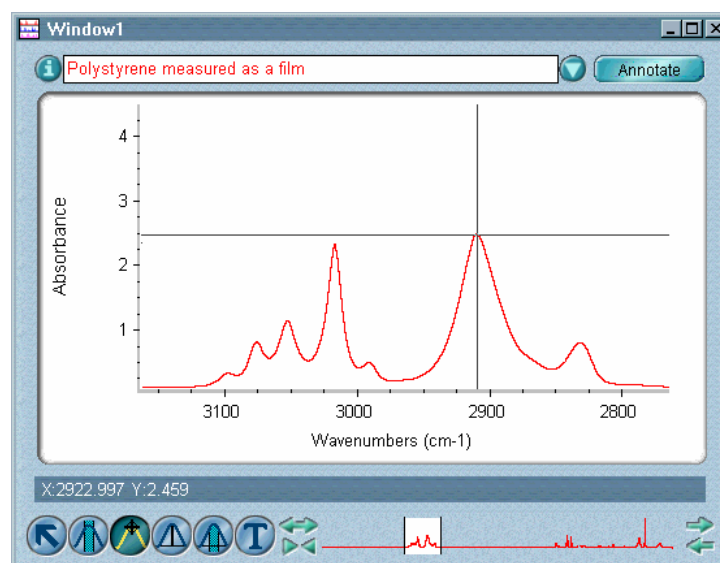
When you are finished measuring peak areas, you can print the spectrum with all the area (and other) annotations by using Print in the File menu.

**Note** When you save a spectrum, its annotations are saved and will be displayed when you later open the spectrum. ▲



**Spectral cursor tool**

Use the spectral cursor tool to see the X and Y values of points in a spectrum. For example, you can use the tool to find the height and exact location of a peak. When you use the tool to click in a pane, a pair of thin perpendicular lines, called the spectral cursor, appears:



The intersection of the lines is at or near a point in the spectrum. The X and Y values of this point are shown in the readout above the palette.

By using the Annotate button after positioning the spectral cursor, you can annotate peaks (or other spectral features) with their uncorrected peak heights (Y values). You can then print the spectrum with these peak annotations.

**Note** You can use Options in the Edit menu to specify the text orientation, font and number of decimal places for peak annotations. See “View options” in the “Edit” chapter for details. ▲

If you open another spectrum or select one by using the up or down arrow keys on the keyboard, the spectral cursor is positioned at the same frequency location in that spectrum.

**Note** You can also label a peak with its X or X and Y values using the annotation tool. ▲

The following summary explains the uses of the spectral cursor tool. In each use described, the tool has already been selected.

**Positioning the spectral cursor** – To move the spectral cursor to a point in the selected spectrum, click the point or press the left or right arrow keys on the keyboard until the cursor is at the desired location. It does not matter if you click above or below the spectrum; only the X value is used. The left arrow key moves the cursor to the left; the right arrow key moves the cursor to the right.

If you find it difficult to position the cursor exactly where you want it, first expand the display of the region of interest by using the view finder or selection tool.

To position the spectral cursor at the top of a peak in a selected spectrum in absorbance, Kubelka-Munk or log (1/R) units, hold down the Shift key and click near the peak. The X location and Y value of the peak appear in the readout above the palette. If the spectrum is in % transmittance, photoacoustic or % reflectance units, you can position the cursor at the bottom of a peak using the same technique.

You can use the Annotate button to label the point with its height (Y value). This is explained in the next procedure.

**Labeling peaks with their uncorrected heights** – Follow these steps:

**1. Position the spectral cursor by clicking the tip of the peak (or other spectral feature) you want to label.**

You can hold down the Shift key when clicking a peak to automatically place the cursor at the top of the peak.

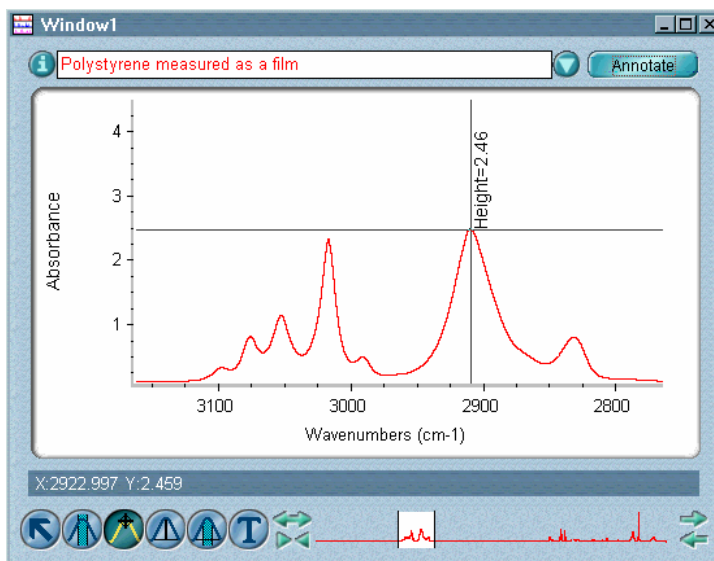
You can start over by positioning the spectral cursor at a different point before clicking the Annotate button in the next step. (After you click the Annotate button, you will need to delete the annotation if you want to start over.)

**2. Click the Annotate button to the right of the title box.**

**Note** The Annotate button is available only if Annotation is turned on in the Display Setup dialog box. ▲

The uncorrected peak height (Y value) appears as an annotation near the peak (see the following example).

You can position the annotation by using the annotation tool.



You can label another peak with its height by repeating steps 1 and 2.

After you click the Annotate button, the annotation remains on the screen when you label another peak or use another tool. The uncorrected peak height is indicated by a vertical line that extends to zero absorbance units (or 100% transmittance).

When you are finished labeling peaks, you can print the spectrum with all the height (and other) annotations by using Print in the File menu.

**Note** When you save a spectrum, its annotations are saved and will be displayed when you later open the spectrum. ▲

### Peak height tool



You can measure the height of a peak from zero absorbance (or 100% transmittance), without regard to the position of the baseline, or from the baseline. The latter measurement is called the “corrected peak height.” The peak height tool lets you find the height of a peak measured from a baseline connecting the low points on either side of the peak (high points are used if the spectrum is in % transmittance). You can adjust the baseline and the peak location to define the peak height you want to measure (this is explained in the procedures that follow).

The tool also finds and displays the X and Y values of the peak and the uncorrected peak height. The uncorrected peak height is the height measured from zero (or from 100% in the case of a transmittance spectrum).

By using the Annotate button after peak height measurements, you can annotate peaks with their corrected heights and then print the spectrum with the annotations.

**Note** You can use Options in the Edit menu to specify the text orientation, font and number of decimal places for annotations. See “View options” in the “Edit” chapter. ▲

**Measuring the height of a peak** – Follow these steps:

**1. Select the spectrum that contains the peak of interest.**

To make it easier to see the peak, you can enlarge the portion of the spectrum that contains the peak by using the view finder or selection tool.

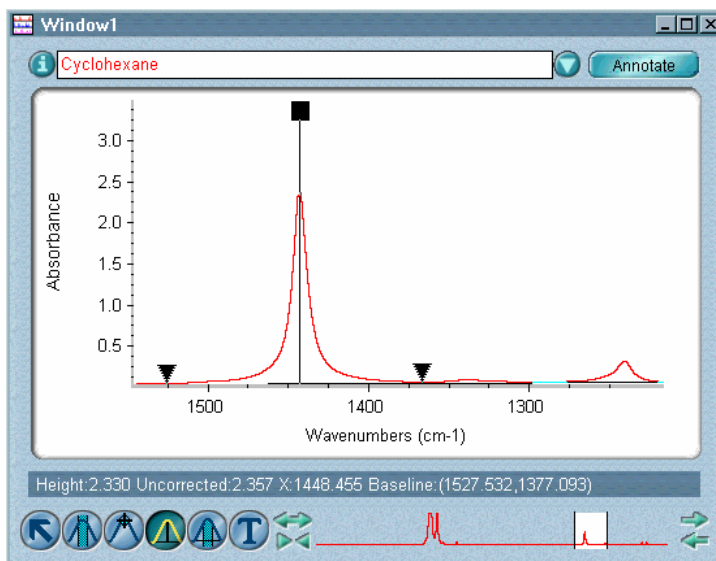
**2. Select the peak height tool.**

**3. Click the top of the peak you want to measure.**

To increase the accuracy of the measurement, hold down the Shift key when clicking to automatically locate the top of the peak.

A vertical line appears at the clicked location (see the following example). At the top of the line is a solid black square that you can drag to the left or right to specify a different peak location. The X value of the line is displayed in the readout above the palette as you drag the square.

The corrected peak height appears in the readout, along with the uncorrected peak height, the X value of the peak and the X values of the baseline endpoints.



A baseline is drawn through the lowest data points (minimum Y values) on either side of the peak. The portion of the vertical line between the top of the peak and the baseline represents the corrected peak height. Two triangular handles on the baseline indicate the baseline endpoints. You can drag these handles to adjust the position of the endpoints.

**Note** If you open another spectrum or select one by using the up or down arrow keys on the keyboard, the height at the corresponding X value in that spectrum is calculated (using a new baseline drawn between endpoints with the same X values as before). ▲

You can use the Annotate button to label the peak with its corrected height. This is explained in the next procedure.

**Labeling peaks with their corrected heights** – Follow these steps:

- 1. Use the peak height tool to measure the height of a peak you want to label.**

You can hold down the Shift key when clicking a peak with the tool to automatically locate the top of the peak.

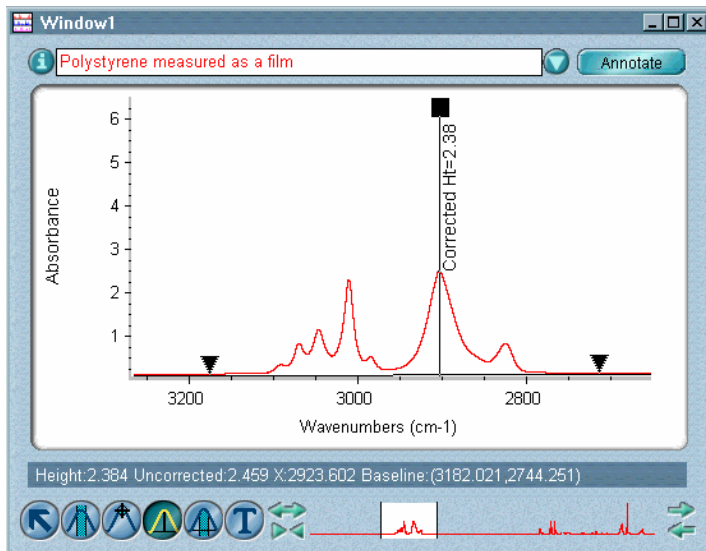
You can start over by measuring the height of a different peak before clicking the Annotate button in the next step. (After you click the Annotate button, you will need to delete the annotation if you want to start over.)

**2. Click the Annotate button to the right of the title box.**

**Note** The Annotate button is available only if Annotation is turned on in the Display Setup dialog box. ▲

The corrected height measurement appears as an annotation near the peak, with a line indicating the baseline used for the measurement.

You can position the annotation text by using the annotation tool.



You can label another peak with its corrected height by repeating steps 1 and 2.

After you click the Annotate button, the annotation remains on the screen when you label another peak or use another tool. The corrected peak height is indicated by a vertical line, and the baseline that defines the height also appears as part of the annotation.

When you are finished labeling peaks, you can print the spectrum with all the annotations by using Print in the File menu.

**Note** When you save a spectrum, its annotations are saved and will be displayed when you later open the spectrum. ▲

**Peak area tool**



Use the peak area tool to find the area under a peak. The area is measured from a baseline connecting the low points on either side of the peak and between the X values of specified points in the peak. (High points on either side of the peak are used for the baseline if the spectrum is in % transmittance). This area is called the “corrected peak area.”

You can adjust the baseline and the region limits to define the peak area you want to measure (this is explained in the procedures that follow).

The tool also finds and displays the uncorrected peak area. The uncorrected area is measured from zero absorbance instead of the baseline. (In a transmittance spectrum, the uncorrected area is measured from 100% transmittance.)

By using the Annotate button after measuring a peak area, you can annotate peaks with their corrected areas. You can then print the spectrum with these annotations.

**Note** You can use Options in the Edit menu to specify the text orientation, font and number of decimal places for peak area annotations. See “View options” in the “Edit” chapter for details. ▲

**Measuring the area under a peak** – Follow these steps:

**1. Select the spectrum that contains the peak of interest.**

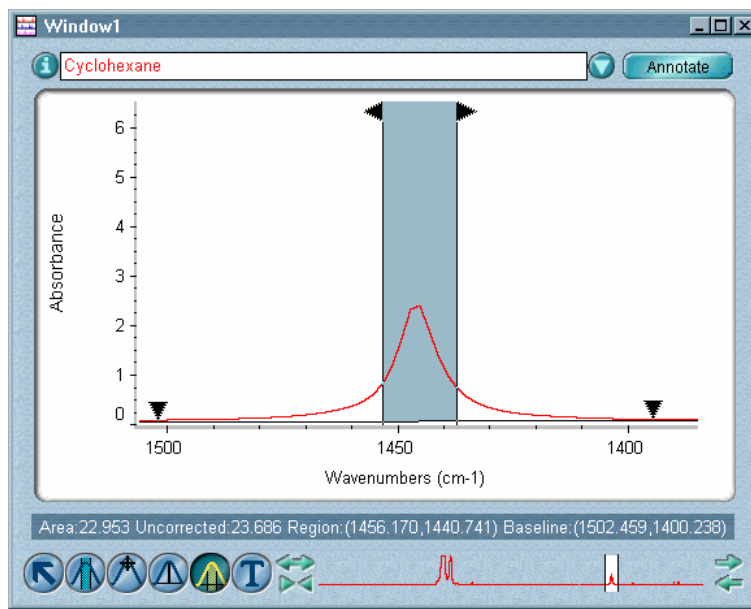
To make it easier to see the peak, you can enlarge the portion of the spectrum that contains the peak by using the view finder or selection tool.

**2. Select the peak area tool.**

**3. Point in the pane to the X value you want to use as the left limit of the area to be measured and press and hold down the mouse button.**

**4. Drag the pointer to a point whose X value you want to use as the right limit of the area and then release the mouse button.**

As you drag the pointer, two vertical lines appear at the limits of the region. When you release the mouse button, the region between the first point and the current pointer location is shaded. See the following example.



At the top of each line is a triangular handle that you can drag to the left or right to change the limit. A baseline is drawn through the lowest data points (minimum Y values) on either side of the peak.

Two triangular handles on the baseline indicate the baseline endpoints. You can drag these handles to adjust the position of the endpoints.

The corrected area is bordered by the spectrum, the X-axis limits of the shaded region and the baseline. In an absorbance spectrum, the uncorrected area is bordered by the X-axis ( $Y=0$ ) instead of the baseline. In a transmittance spectrum, the uncorrected area is measured from 100% transmittance instead of the baseline. The corrected and uncorrected area measurements, limits of the shaded region and X values of the baseline endpoints are displayed in the readout above the palette.

**Note** If you open another spectrum or select one using the up or down arrow keys on the keyboard, the area is calculated for the same region of that spectrum (using a new baseline drawn between endpoints with the same X values as the old endpoints). ▲

You can use the Annotate button to label the peak with its corrected area. This is explained in the next procedure.



**Labeling peaks with their corrected areas** – Follow these steps:

1. Use the peak area tool to measure the area of a peak you want to label.

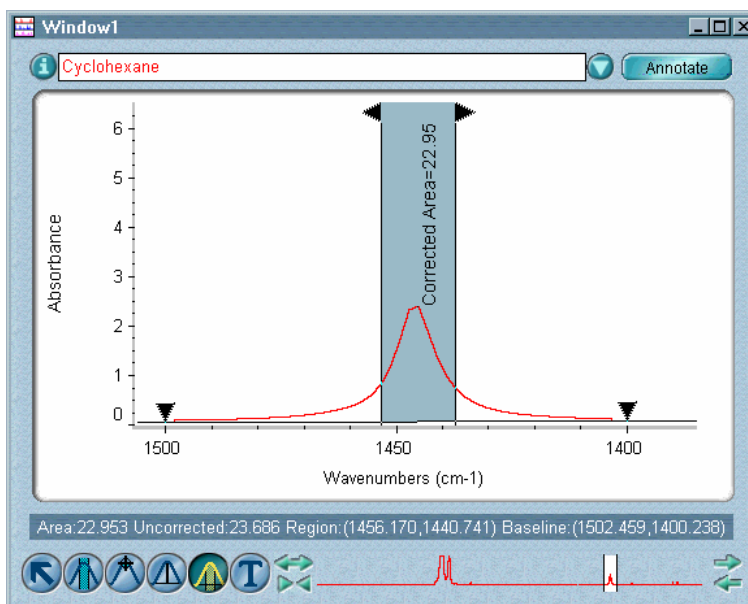
You can start over by measuring the area of a different peak before clicking the Annotate button in the next step. (After you click the Annotate button, you will need to delete the annotation if you want to start over.)

2. Click the Annotate button to the right of the title box.

**Note** The Annotate button is available only if Annotation is turned on in the Display Setup dialog box. ▲

The corrected area measurement appears as an annotation near the peak, with a line indicating the baseline used for the measurement and vertical lines indicating the limits of the measured region.

You can position the annotation text by using the annotation tool.



You can label another peak with its corrected area by repeating steps 1 and 2. After you click the Annotate button, the annotation remains on the screen when you label another peak or use another tool. The corrected peak area is shaded, vertical lines show the frequency limits of the area, and the baseline that defines the area also appears as part of the annotation.

When you are finished labeling peaks, you can print the spectrum with all the annotations by using Print in the File menu.

**Note** When you save a spectrum, its annotations are saved and will be displayed when you later open the spectrum. ▲

**Annotation tool** When selected, the annotation tool lets you perform these operations:



- Add a label
- Edit a label
- Move a label
- Delete a label
- Move sampling information

**Note** The annotation tool is available only when the Annotation option is turned on in the Display Setup dialog box. See “Displaying annotation” in the “View” chapter for details. ▲

**Note** You can use Options in the Edit menu to specify the text orientation, font and number of decimal of places for labels. See “View options” in the “Edit” chapter. ▲

When you save a spectrum, its annotations are saved and will be displayed when you later open the spectrum. The annotations also become part of the spectrum's collection and processing information and can be viewed in table form with the Annotation button.

The following summary explains the uses of the annotation tool. In each use described, the tool has already been selected.

**Adding a label** – Follow these steps:

**1. Click a location for the label.**

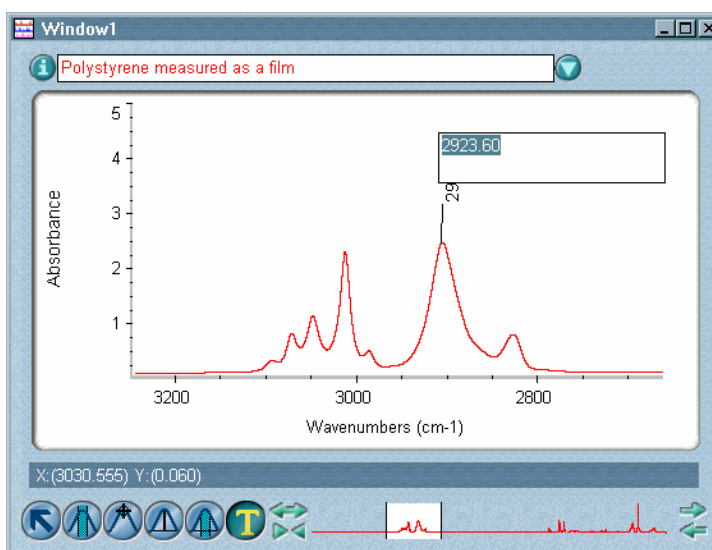
It doesn't matter if you click above or below the spectrum; only the X value of the clicked point determines which point in the spectrum is labeled.

**Note** You can more accurately label the top of a peak by holding down the Shift key when you click near the peak. ▲

The type of label that appears depends on the current setting of X And Y Values in the Display Setup dialog box. See “Specifying how to display annotation” in the “View” chapter for more information.

- If X And Y Values is off, a label shows the X value of the point you clicked. The text of the label is selected to allow you to edit it.
- If X And Y Values is on, the label shows both the X and Y values of the point and the label text is selected.

If Connect To Spectrum is turned on in the Display Setup dialog box, a line is drawn connecting the label to the spectrum. See “Specifying how to display annotation” in the “View” chapter for more information on the Connect To Spectrum option.



## 2. Edit the label text if desired.

If you don't want to keep the label, delete all the text. Editing labels is explained later in this section.

**Note** You can use Options in the Edit menu to specify the orientation and font for labels. See “View options” in the “Edit” chapter for details. ▲

## 3. Press Enter.

The label appears with the specified orientation. You can then click a new location to add another label.

**Editing a label** – Follow these steps:

**1. Click the text of the label.**

The text becomes selected.

**2. Type the desired new text.**

**3. Press Enter.**

**Moving a label** – Drag the label text to the desired location. When you release the mouse button, the text is selected and can be edited. To keep the current text, press Enter.

**Note** A label created using Find Peaks in the Analyze menu will always be connected to the spectrum with a line if you move the label away from the spectrum. ▲

**Deleting a label** – Follow these steps:

**1. Click the text of the label to select it.**

**2. Press Backspace or Delete.**

**3. Press Enter.**

**Moving sampling information** – Drag the text to the desired location in the pane.

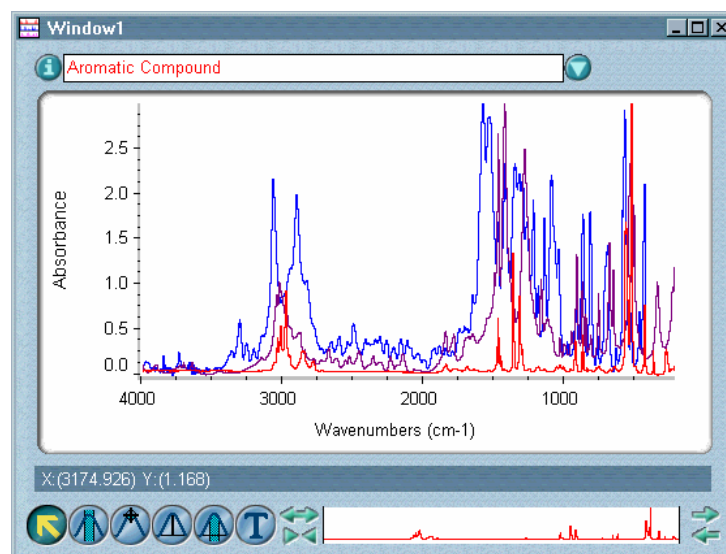
## **Overlaying and stacking spectra**

There are two ways of displaying spectra in a spectral window. You can overlay them so that their panes are on top of one another, similar to a neat pile of transparent sheets. You can also stack them so that their panes appear above one another on the screen. In either case, only one spectrum can be displayed in a pane.

To overlay spectra that are currently stacked, use **Overlay Spectra** in the **View** menu. After you use the command, its name changes to **Stack Spectra**. To stack spectra that are currently overlaid, use the **Stack Spectra** command. See “Stacking or overlaying spectra” in the “View” chapter for more information.

### Overlaying spectra

When you overlay spectra in a spectral window (see the example below), their panes are on top of one another, similar to a neat pile of transparent sheets.



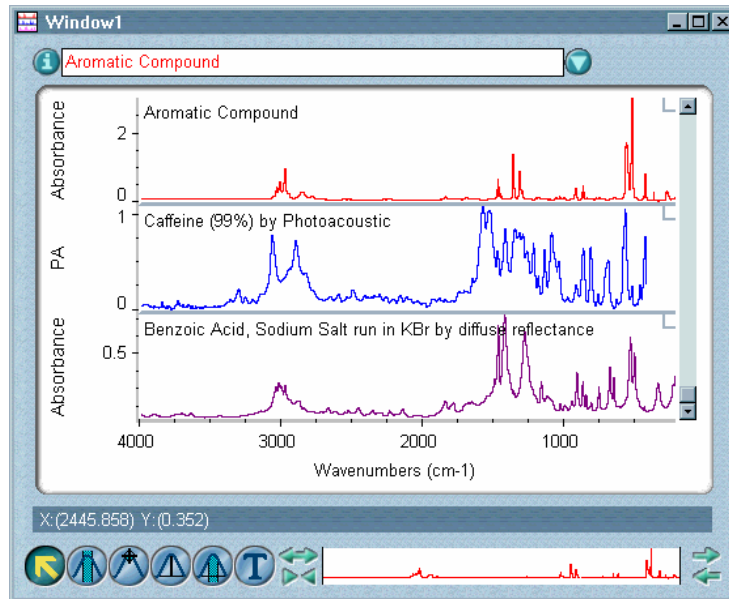
Overlaying spectra lets you see significant differences in their spectral features. (Expanding the display can help you see small differences in a particular region.)

To hide an overlaid spectrum so that it doesn't appear on the screen, use **Hide Spectra** in the **View** menu. See “Hiding spectra” in the “View” chapter for details.

### Stacking spectra

When you stack spectra in a spectral window (see the following example), their panes appear above one another on the screen.

The title of each stacked spectrum is shown in the spectrum's pane.

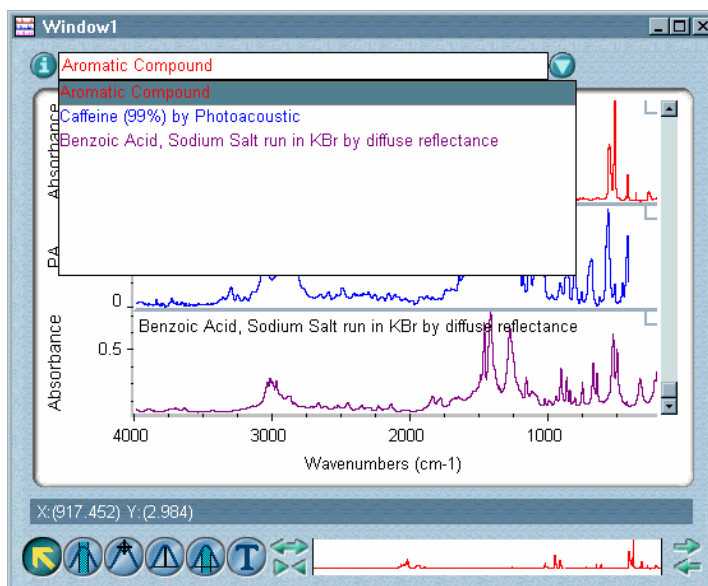


Only one spectrum can be displayed in a pane. Stacking spectra is useful when you are comparing spectra that are significantly different. For example, stacking the library spectra found in a spectral search can make it easier to decide which spectrum most closely matches the unknown sample.

When you stack spectra, you set the number of panes in the spectral window by using Display Setup in the View menu (see “Specifying how to stack spectra” in the “View” chapter for details). There can be more panes in the window than there are spectra, resulting in one or more empty panes. There can also be more spectra in the window than there are panes. In this case some spectra may be out of view “above” or “below” the panes. You can scroll spectra into view or into an empty pane (this is explained below).

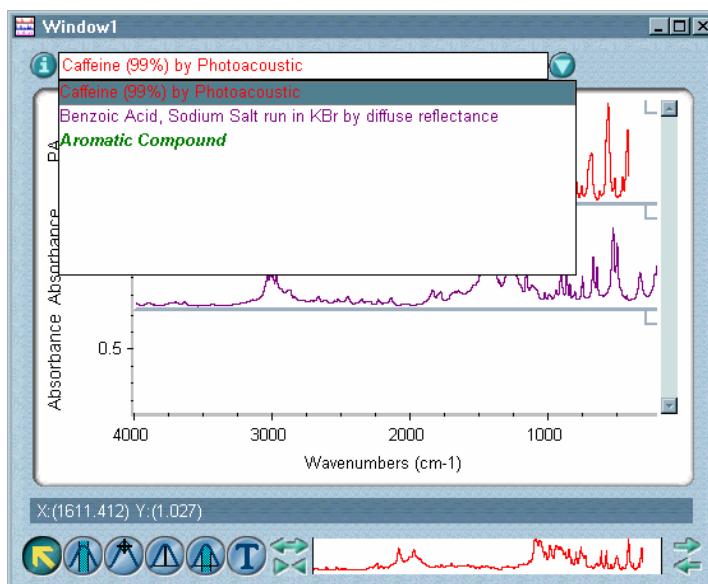
Each pane in the stack has its own Y-axis. Any X-axis adjustments that you make using the view finder will affect all of the spectra in the window.

**Displaying a list of stacked spectra** – Click the arrow at the right end of the title box to see a list of all the spectra in the window, including those out of view (see the following example). The spectrum titles appear in the list in order from top to bottom.



**Hiding a stacked spectrum** – Use Hide Spectra in the View menu to hide a stacked spectrum so that it doesn't appear on the screen (see “Hiding spectra” in the “View” chapter for details). When a stacked spectrum is hidden, its title appears in the font specified for the titles of hidden spectra in the View options. The default font for displaying the titles of hidden spectra is italic. (See “Specifying fonts for displayed text” in the “Edit” chapter.)

In this example, the spectrum titled “Aromatic Compound” is hidden.



When you hide a stacked spectrum, any displayed spectra below it move up one pane so that the pane which contained the hidden spectrum is filled. Locked panes are skipped over as the spectra move up.

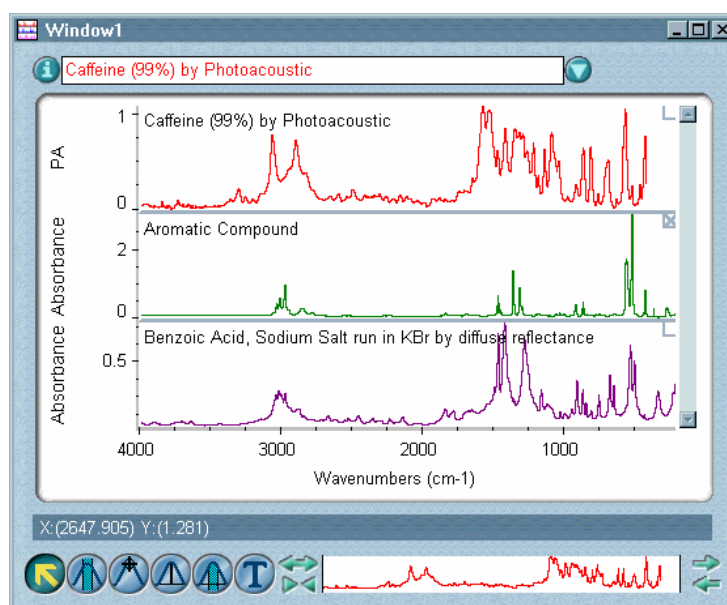
When you hide a selected spectrum, another spectrum in the window (if there is one) becomes selected instead.

To make a hidden spectrum visible, select the spectrum by clicking its title in the list of titles.

**Locking a spectrum in its pane** – Click the small box in the upper-right corner of the pane. An X appears in the pane lock when the pane is locked; if there is no X in the pane lock, the pane is not locked.

In this example, the middle pane is locked.

When a spectrum is locked in a pane, no other spectrum can be displayed in that pane.



Locking panes is useful for maintaining the position of a spectrum in the stack when hiding or scrolling spectra (explained later in this section).

You can perform operations on a spectrum in a locked pane just as you would on a spectrum in an unlocked pane.

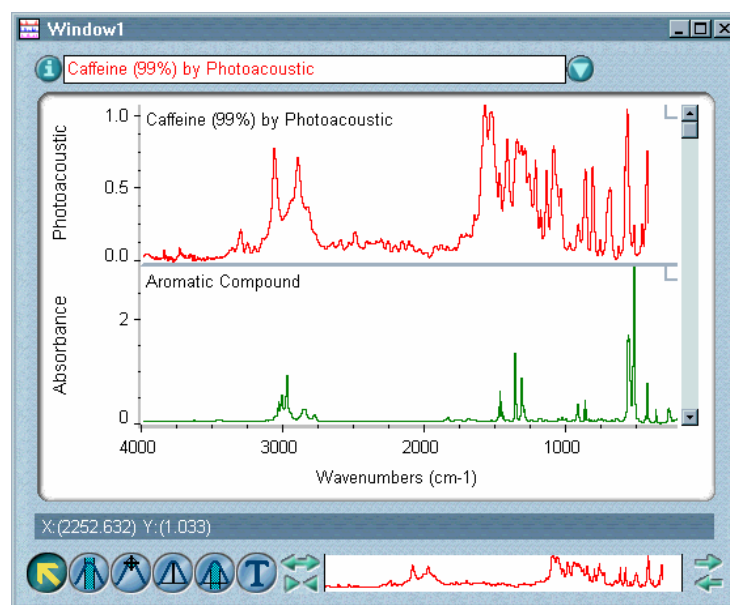
To unlock a pane, click its pane lock.

**Scrolling stacked spectra** – Use the scroll bar at the right of the pane to display spectra currently out of view above or below the panes. Clicking the upper scroll arrow moves the spectra down one pane, and clicking the lower scroll arrow moves the spectra up one pane. You can also drag the scroll box up or down to display spectra that are out of view. If all the spectra are displayed, the scroll bar is unavailable.



In the following example, the spectral window contains three spectra and two panes. The last spectrum is out of view below the panes. Notice that the scroll bar is available and contains a scroll box (currently at its highest position within the scroll bar).

You can also use the up and down arrow keys on the keyboard to scroll spectra into view. First select the scroll bar by clicking the scroll box and then press the up arrow key to move the spectra down one pane or the down arrow key to move the spectra up one pane.



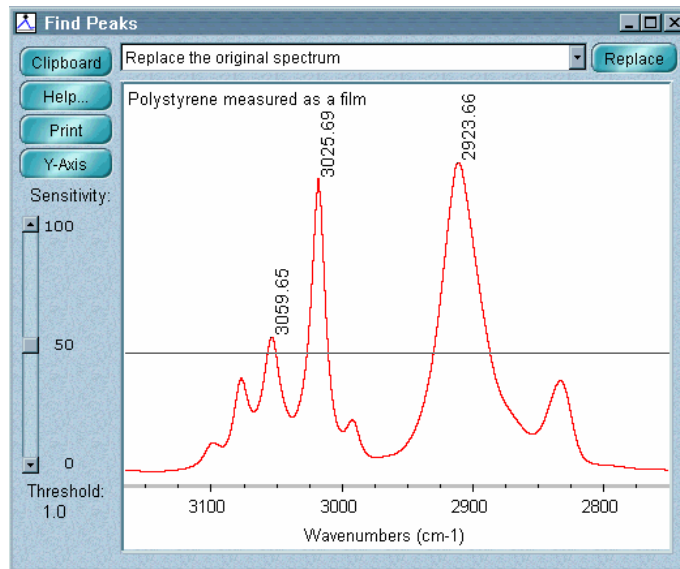
If a pane containing a spectrum is locked, that spectrum does not move when you scroll. As the other spectra move up or down during scrolling, the locked pane is skipped over.

The order of spectra in the list of titles is not affected by scrolling unless one or more panes are locked. Since locked panes are skipped over as spectra are scrolled up or down, the order of the spectra in the window changes. When you are through scrolling, the new order is shown in the title box.

## Task windows

When you use some OMNIC commands, a special window is displayed to let you see the progress of an operation or to let you interact with the software during the operation. These windows are called task windows. In each task window one or more spectra are displayed.

For example, when you use Find Peaks to find peaks in a spectrum, the following task window appears. Like the other task windows, this window is unique and contains all the features needed to complete the operation.



When the operation is finished, you can use the window selection box at the top of the task window to add the resulting spectrum to a spectral window or replace the original spectrum in its window. To select one of these options, click the arrow to the right of the window selection box and then click the desired option in the list that appears.

When the result spectrum is placed in a spectral window, an asterisk appears at the beginning of the spectrum title so you can tell it apart from the original spectrum.

\*Polystyrene measured as a film

If you perform an operation on the result spectrum with a command that uses a task window, another asterisk will appear at the beginning of the spectrum title if you place the result of that operation in a spectral window.

\*\*Polystyrene measured as a film

**Note** You can close a task window by clicking the Close button (if available) in the upper-right corner of the window or by double-clicking 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). ▲

**Note** When a task window is maximized, it shares a title bar with the OMNIC window. ▲

# File

The File menu includes commands that let you perform these operations:

To do this...	Use this command...
Retrieve spectra saved on a disk.	Open
Save a spectrum on a disk.	Save
Save a spectrum using a new filename.	Save As
Save a group of spectra.	Save Group
E-mail the selected spectra.	Mail Spectra
Sign a file.	Sign File
Verify a digital signature.	Verify File
Open a configuration saved on a disk.	Open Configuration
Save the current configuration.	Save Configuration As
Log into OMNIC as the current user.	Log In
Add your name as a user of OMNIC.	Add User Name
Turn the log-in feature on or off.	Enable OMNIC Log-In
Open a log for recording operations.	Open Log
Print or plot the results of your work.	Print
Set up the system printer.	Printer Setup
Delete files from a disk.	Delete Files
Exit OMNIC.	Exit

## Opening spectra

Use Open in the File menu to retrieve one or more spectra or a group of spectra stored in spectral data files on a disk. When you open a spectrum, OMNIC displays the spectrum in the active spectral window or in a new spectral window if no spectral window currently exists. See “Saving a group of spectra” for information on saving spectra as a group.

You can use Open to open spectra that were saved using OMNIC or spectra that are in another format, or “file type.”

The normal DOS extensions used for each file type are shown in the following table (other extensions are allowed).

File Type	Extension	Comments
Spectra	.SPA	This is the default type.
Spectral Groups	.SPG	This type can contain multiple spectra that were saved together in one file.
JCAMP-DX	.JDX	This type can contain multiple spectra that were saved together in one file.
PCIR	.IRD	
Nicolet SX/DX	.NIC or .SPC	
CSV Text	.CSV	
PeakSolve	.0??	The ?? in the extension represents the sequential number of the spectrum. For example, if you had five PeakSolve files, their filenames would have the extensions .001, .002, .003, .004 and .005.
GRAMS/386 or GRAMS/AI	.SPC or .GLD	An .SPC file can contain multiple spectra that were saved together in one file.
Perkin-Elmer	.SP	
Mattson	.IGM, .ABS, .DRT, .TRN, .SBM or .RAS	
Spectacle	.IRS, .SDA, or .UVD	

The available file types are shown in the List Files Of Type drop-down list box in the Open dialog box.

**Note** To list all the files in the indicated directory, select All Files (\*.\*) from the List Files Of Type drop-down list box in the Open dialog box. ▲

## Opening a CSV text file

CSV (comma-separated values) text files contain data in the form of pairs of X and Y values (the values can be evenly or unevenly spaced). If you save a spectrum as a CSV file, you can process the data using a spreadsheet program or other program that uses the CSV file format. You can then use OMNIC to open and display the file as a spectrum and save it if desired as a spectral data file (with the extension .SPA) with the axis units you specify.

The CSV file must meet the following requirements to be opened:

- It is a text file (with the extension .CSV) consisting of a list of pairs of X and Y values.
- Each pair is on a separate line and each line is ended by pressing the Return or Enter key.
- There is a comma, tab, space or line feed between the X and Y values.
- The X values are in increasing order.
- The X and Y values are floating-point decimal numbers (decimal point in any position), integers, numbers in scientific notation, or a combination of these.

If the spacing between consecutive X values is not constant, the software interpolates the data where necessary to produce a spectrum whose spacing is constant.

**Note** CSV files do not contain the kinds of information included in the Collection And Processing Information window for a spectrum. ▲

Here is an example of a portion of a list of X,Y pairs from a CSV file that meets these requirements:

```
3053.8,1.59
3058.4,1.90
3063.0,1.83
3067.6,1.53
3072.2,1.45
```

When you choose OK in the Open dialog box to open the CSV file, the Parameters dialog box allows you to set parameters for creating the spectrum. The table below describes them and the readouts that appear in the dialog box.

Feature	Description
Spectrum Title	The title for the spectrum.
X Units	The X-axis format of the spectrum.
Y Units	The Y-axis format of the spectrum.
Resolution	The resolution of the spectrum. The default value is the resolution value available in OMNIC that is closest to the resolution of the data in the file. You can select a different value. The default resolution is obtained by dividing the spectral range by the number of data points and then multiplying the result by two.

The First X and Last X readouts show the first and last X values, respectively, of the spectrum.

The Data Points readout shows the number data points that will be in the spectrum when the file is read and, in parentheses, the number of data points in the CSV file. These two values are different when the selected resolution does not correspond to the data point spacing in the CSV file.

The settings available in the X Units drop-down list box are described in the table below.

Setting	X-Axis Format
Undefined	No X-axis unit is displayed.
Wavenumbers	Wavenumbers.
Data Points	Data points.

The settings available in the Y Units drop-down list box are described in the following table.

<b>Setting</b>	<b>Y-Axis Format</b>
Undefined	No Y-axis unit is displayed.
Energy	Instrument energy response.
Gram-Schmidt	Intensity.
% Reflectance	Percent reflectance.
Log(1/R)	Log (1/R) units.
Concentration (ppt)	Concentration in parts per thousand.
Real/Imaginary	Real/imaginary pair.
Single Beam	Single-beam format.
% Transmittance	Percent transmittance.
Absorbance	Absorbance.
Digitizer	Digitizer output.
Emittance	Emittance units.
Kubelka-Munk	Kubelka-Munk units.
Reflectance	Reflectance.
Volts	Volts.
Transmittance	Transmittance.
Frequency (MHz)	Frequency in megahertz.
Frequency (GHz)	Frequency in gigahertz.
Photoacoustic	Photoacoustic units.
Blackbody	Radiance.
Phase	Phase angle in radians.
Intensity	(Chemigram) intensity.



You can click the More button in the Parameters dialog box to display another dialog box that lets you set additional parameters (described in the next table). *These parameters record information about the data for future reference; they do not affect the conversion of the data.*

**Note** These parameters may not be applicable to files containing values for near-IR data collected using a dispersive spectrometer. ▲

Parameter	Description
Apodization	The apodization type for the spectrum.
Phase Correction	The phase correction used for the spectrum.
Sample Spacing	The sample spacing of the spectrum (the number of zero crossings of the reference laser).
ZPD Point	The zero path difference point for the spectrum.
Resolution Points	The number of resolution points; that is, points after the ZPD (zero path difference) point.
Transform Points	The number of transform points for the spectrum.
Number Of Scans	The number of scans for the spectrum.
Gain	The electronic gain for the spectrum.

## Opening a spectrum by dragging its file into a spectral window

You can quickly open one or more spectra by dragging their files from a folder into a spectral window. Follow these steps:

- 1. Use Computer, My Computer or Windows Explorer to display the spectral data files you want to open.**
- 2. Arrange the windows on the screen so that the spectral data files and the spectral window are visible.**

If no spectral window exists, create one by using New Window in the Window menu. See “Creating a new spectral window” in the “Window” chapter for details.



**3. Select and drag the files to the spectral display area of the spectral window.**

To select one file, click its filename. You can select more than one file by holding down the Control key or Shift key while clicking the filenames.

The spectra are opened in the spectral window. The files remain in their original locations.

## Opening a spectrum by choosing its filename from the File menu

A list of the most recently opened spectral data files appears at the bottom of the File menu of OMNIC. You can open a file in this list by choosing it from the menu.

### — How to ➔

Open a spectrum or spectra using the Open command

**1. If Put Opened Spectrum In New Window is off in the File options (available through Options in the Edit menu), select the spectral window in which you want to display the spectra.**

If only one spectral window exists, that is the selected window.

If Put Opened Spectrum In New Window is on or if no spectral window exists, the spectra will be displayed in a new spectral window. See “Placing opened spectra into new spectral windows” in the “Edit” chapter for more information.

**2. Choose Open from the File menu.**

The Open dialog box lists files of the Spectra (\*.SPA) file type. You can list files of other types by selecting a type from the List Files Of Type drop-down list box.

**3. Type the name of the file you want to open, or locate and select one or more files.**

To select one file, click its filename. To select more than one, hold down the Control key and click the desired filenames. You can change directories or drives to locate the files.

**Note for DS systems**

If Prevent Changing Directories When Opening Files is selected in the system policies, you cannot change directories or drives to locate files to open. ▲

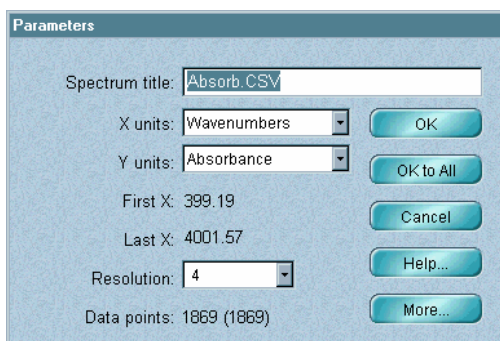
Whenever possible a “preview” image of the spectrum appears in the dialog box. If you select multiple files of this type, an image of the spectrum you selected first appears.

**Note**

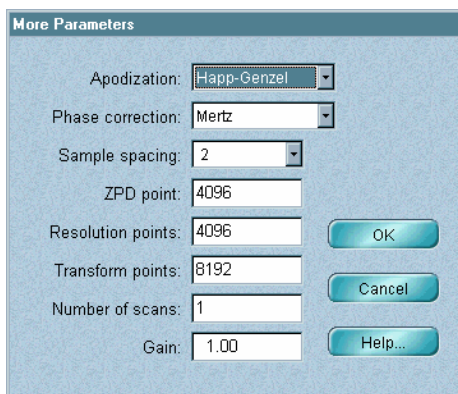
You can specify a default directory in the File options (available through Options in the Edit menu). (If you have the DS option, the directory is specified by the Directory For Spectral Data system policy.) ▲

**4. Choose OK.**

If you are opening a CSV text file, the Parameters dialog box lets you set several parameters that affect the conversion of the data or that record information about the spectrum.



If the file you are opening contains evenly spaced data points, you can use the default settings. If the file contains unevenly spaced data points, set the parameters. Use the More button to display additional parameters and set them.



When you are finished setting the parameters in a dialog box, choose OK. If you are opening more than one CSV file, the Parameters dialog box appears for each file. You can set the parameters for each file individually and choose OK each time, or you can choose OK To All to accept the current settings for all the files at once.

Depending on the software option settings and whether a spectral window is open, the spectrum or spectra you open may appear in the active spectral window or in a new window. The spectrum that is opened last is selected and can immediately be used in other operations.

## Saving a spectrum

Use Save in the File menu to save a spectrum in a file on a disk using the spectrum's current filename. (If the spectrum does not have a filename, you will be asked to enter one.)

**Note** The default extension used to save a spectrum is .SPA. To specify that a spectrum be saved using another file type, use the Save As command. See “Saving spectra using new filenames” for details. ▲

### — *How to* ➔

Save a spectrum

### **Note for DS systems**

You may be prompted to digitally sign a file; follow the instructions that appear on the screen. If Require Signature When Saving Spectrum is selected in the system policies, the Save As dialog box will appear (see step 3). If you want to sign the file, turn on Use Digital Signature. ▲

- 1. Select the spectrum.**
- 2. Choose Save from the File menu.**

If the spectrum has a current filename, the spectrum is saved on the disk using the same name and the operation is finished. If the spectrum does not have a current filename, the Save As dialog box appears.

**3. If the Save As dialog box appears, type a filename and select a directory in which to save the spectrum.**

To save the spectrum using a file type other than Spectra (OMNIC .SPA format), select the desired type from the Save File As Type drop-down list box and type the appropriate extension at the end of the filename. Each listed file type shows the correct extension.

**Note** You can specify a default directory for this operation in the File options (available through Options in the Edit menu). See “Specifying directories” in the “Edit” chapter. (If you have the DS option, the directory is specified by the Directory For Spectral Data system policy.) ▲

If you want the spectrum saved so that it can be opened later but not changed and saved with the changes, turn on the Read Only check box near the lower-left corner of the dialog box.

**4. Choose OK.**

## **Saving spectra using new filenames**

Use Save As in the File menu to save one or more spectra in files on a disk using new filenames. In addition to saving spectral data in regular OMNIC files (with the extension .SPA), you can select other file types such as PCIR, JCAMP-DX, Nicolet SX/DX, TIFF, CSV (comma-separated values), WMF (Windows metafile), Mattson or GAML. The available file types are shown in a drop-down list box in the Save As dialog box.

The TIFF and WMF file types save only the graphical information of the spectrum; you can open these files using an appropriate graphics program.

The CSV file type saves only the spectral data in a numerical form; you can open this type of file using an appropriate spreadsheet program. (You can also open this file type using OMNIC.)

If you save data in a CSV text file, only the selected spectral region (or displayed region if no region is selected) is saved.

**— How to ➡**

Save spectra using new filenames

**Note for DS systems**

You may be prompted to digitally sign a file; follow the instructions that appear on the screen. If you want to sign the file, turn on Use Digital Signature in the Save As dialog box. ▲

**1. Select the spectra.**

If you are saving data in a CSV text file, display or select the spectral region you want to save by using the view finder or region tool. Only the selected region, or displayed region if no region is selected, will be saved.

If you are saving data in a Windows metafile, there is no need to select a spectrum; all the spectra in the spectral window will be saved.

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

The Save As dialog box appears.

**3. Type a filename for the first spectrum in the File Name text box.**

You can click the Set Filename To Title button to assign the spectrum title, shown in the yellow box, as the filename.

To save the spectrum using a file type other than Spectra, select the desired file type from the Save File As Type drop-down list box and type the appropriate extension at the end of the filename. Each listed file type shows the correct extension.

**4. Select a directory in which to save the spectrum.**

**Note** You can specify a default directory in the File options (available through Options in the Edit menu). See “Specifying directories” in the “Edit” chapter. (If you have the DS option, the directory is specified by the Directory For Spectral Data system policy.) ▲

5. **If you want the spectrum saved so that it can be opened later but not changed and saved with the changes, turn on the Read Only check box near the lower-left corner of the dialog box.**

6. **Choose Save.**

If there are no more selected spectra to save, the procedure is finished. If there is another spectrum to save, the Save As dialog box reappears.

7. **Repeat steps 3 through 6 for the next spectrum you are saving.**

Continue in this way until all the selected spectra are saved. You can choose Cancel to cancel the save operation for the current spectrum and continue with the next spectrum.

## **Saving a group of spectra**

Use Save Group in the File menu to save more than one spectrum as a group in one file having the file extension .SPG. You can open the group later by using Open in the File menu.

### **— How to —>**

Save a group of spectra

1. **Select the spectra you want to save as a group.**

All the spectra must be in the same spectral window. To select more than one spectrum, click the first spectrum with the selection tool and then hold down the Control key and click each additional spectrum you want to select. Then release the Control key. You can also choose Select All from the Edit menu to select all the spectra in the window.

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

The Save Group dialog box appears. This is a standard Windows dialog box. For more information on using this type of dialog box, see your Windows documentation.

3. **Type a filename for the group.**

#### 4. Select a directory in which to save the group.

**Note** You can specify a default directory in the File options (available through Options in the Edit menu). See “Specifying directories” in the “Edit” chapter. (If you have the DS option, the directory is specified by the Directory For Spectral Data system policy.) ▲

#### 5. If you want the group saved so that it can be opened later but not changed and saved with the changes, turn on the Read Only check box near the lower-left corner of the dialog box.

#### 6. Choose Save.

Tips for saving a group of spectra:

- Save Group is useful for saving a number of related spectra in a single file. For example, various spectra obtained by running a sample as a split mull and other spectra collected using a KBr disk could be saved as a group. You could also save single-beam background and sample spectra as a group before reprocessing them.

## E-mailing spectra

Use Mail Spectra in the File menu to compose and send an e-mail message with the selected spectra as attachments. The spectra must be already saved.

### ■ *How to* ➡

E-mail spectra

#### 1. Select the spectra you want to send.

All of these spectra must be in the same spectral window and must be already saved.

To select more than one spectrum, click the first spectrum with the selection tool and then hold down the Control key and click each additional spectrum you want to select. Then release the Control key.

You can also choose Select All from the Edit menu to select all the spectra in the window.

## 2. Choose Mail Spectra from the File menu.

Your e-mail application displays a window. (If any of the selected spectra are not saved, you are prompted to save them before the e-mail application window appears.)

## 3. Compose a message and send it.

See the documentation that came with your e-mail application if you need help. The spectra, which were attached automatically, are sent with the message.

## Signing a file

If you have the DS option, you can use Sign File in the File menu to digitally sign files that contain spectra, spectral groups, experiments, configurations, macros, maps or series data sets. If you sign a spectral group file, each spectrum contained in the file is signed.

The visible portion of a digital signature consists of a user name, a date and a stated reason for signing. A digital signature also contains encrypted information that lets you detect whether the file has changed since it was signed.

When you sign a spectral data file, a record of when the file was signed and who signed it is added to the spectrum's collection and processing information. (See "Collection and processing information" in the "About the Display" chapter for more information.) For a map you can view this type of information by using Show Map Info in the Atlas menu.

After you sign a file, you can verify the signature by using Verify File in the File menu. See "Verifying a digital signature" for details.

### ■ *How to* ➔

Sign a file

#### 1. Choose Sign File from the File menu.

The Open File For Signature dialog box appears.



## 2. Locate and select the desired files.

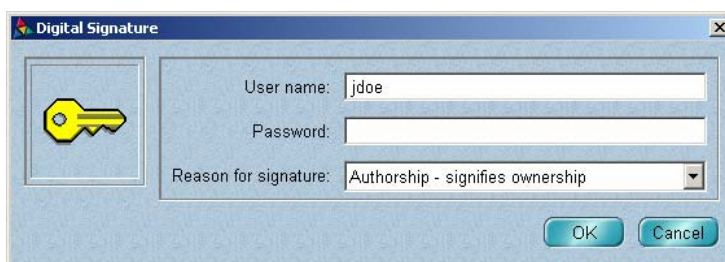
To select multiple files, use standard Windows techniques, such as holding down the Ctrl or Shift key when clicking files.

### Note for DS systems

If Prevent Changing Directories When Opening Files is selected in the system policies, you cannot change directories or drives to locate a file to open. ▲

## 3. Choose Open.

The Digital Signature dialog box appears. Here is an example:



## 4. Verify that the correct user name appears in the User Name text box.

Only the currently logged-in user may sign a file.

## 5. Type your password in the Password text box.

## 6. Select the appropriate reason for signing from the Reason For Signature drop-down list box.

The listed reasons (Review, Approval, Responsibility and Authorship) are provided for meeting requirements described in the document titled *OMNIC Software: 21 CFR Part 11 Compliance* in the “Regulatory Considerations” section of your *FT-IR Spectrometer Validation* or *ValPro System Qualification* handbook. See that document for more information.

You may also be able to type a custom signature meaning in the Reason For Signature box.

**7. Choose OK.**

A message states that the signing was successful.

**8. Choose OK.**

## Verifying a digital signature

### — How to —➔

If you have the DS option, you can use Verify File in the File menu to verify that a file has been digitally signed. You can verify signatures for files that contain spectra, experiments, configurations or macros.

Sign a file

**1. Choose Verify File from the File menu.**

The Open File To Verify Signature dialog box appears.

**2. Locate and select the desired file.**

You can verify signatures for files that contain spectra (.SPA files), experiments (.EXP files) or configurations (.CON files).

**Note for DS systems**

If Prevent Changing Directories When Opening Files is selected in the system policies, you cannot change directories or drives to locate a file to open. ▲

**3. Choose Open.**

If the file has been digitally signed, a message provides information about the signature; for example, the name of the person who signed the file.

If the file has not been digitally signed, a message says that no signature was found.

**4. Choose OK.**

## Signing the selected spectra

If you have the DS option, you can use Sign Spectra in the File menu to sign the selected spectra in the active spectral window.

The visible portion of a digital signature consists of a user name, a date and a stated reason for signing. A digital signature also contains encrypted information that lets you detect whether the file has changed since it was signed.

When you sign a spectrum, a record of when the file was signed and who signed it is added to the spectrum's collection and processing information.

After you sign a spectrum, you can verify the signature by using Verify File in the File menu.

### ■ *How to* ➔

Sign the selected spectra

#### 1. Choose Sign Spectra from the File menu.

- If all of the selected spectra have been signed and saved, the Digital Signature dialog box appears. Go to the next step.
- If a selected spectrum has never been saved, a message informs you. Choose OK and then save the spectrum using the Save As dialog box that appears. When you are finished, the Digital Signature dialog box appears. Go to the next step.
- If an unsigned selected spectrum has been changed since it was last saved, a message informs you. Choose OK to save the spectrum. The Digital Signature dialog box appears. Go to the next step.
- If a signed selected spectrum has been changed since it was last saved, a message informs you. Choose OK. A message asks whether to replace the signed file. Choose Yes. The Digital Signature dialog box appears. Go to the next step.

#### 2. Verify that the correct user name appears in the User Name text box.

Only the currently logged-in user may sign a file.

3. **Type your password in the Password text box.**
4. **Select the appropriate signature meaning from the Reason For Signature drop-down list box.**

The listed meanings may vary depending on the security policies of your system and may include Authorship, Approval, Review, Revision or others. These meanings can be used for meeting requirements described in the document titled *OMNIC Software: 21 CFR Part 11 Compliance*. See that document for more information.

You may also be able to type a custom signature meaning in the Reason For Signature box.

5. **Choose OK.**

A message states that the signing was successful.

6. **Choose OK.**

## Opening a configuration

Use Open Configuration in the File menu to open a configuration that is stored on a disk. When you open the configuration, the OMNIC menus and toolbar (if displayed) appear with the features specified by the configuration. In addition, the options in the Options dialog box are set as specified by the configuration. This makes it easy to set up the software according to your preferences without having to set individual parameters. See “Customizing the OMNIC menus” and “Customizing a toolbar” in the “Edit” chapter and “Saving a configuration” in this chapter for details on creating and saving a configuration that sets up the software according to your preferences.

### Note for DS systems

Access to standard menu items is controlled by the Security Administration software, regardless of the settings in the current configuration or menu changes you make with Edit Menu in the Edit menu. ▲

A number of example configuration files are included with your OMNIC software and described in the following table. These files are located in the Param directory within the OMNIC directory.

Configuration Filename	Description
SCANPLOT.CON	A very simple configuration that allows only data collection, printing and a few other operations.
BASCFTIR.CON	A basic configuration that includes common FT-IR functions.
COMPLETE.CON	A complete configuration with all of OMNIC's features, including the toolbar.
OMNIC21.CON	A configuration whose menus are similar to those of OMNIC 2.1. The toolbar is not available.
EZOMNIC.CON	A configuration that contains only the limited set of features.

### ■ *How to* ➔

Open a configuration

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

The Open Configuration dialog box lists the available configuration files (with the extension .CON). The provided example configuration files are in the Param directory within the OMNIC directory.

#### 2. Type the name of the file you want to open, or locate a file and select it by clicking its filename.

#### Note for DS systems

If Prevent Changing Directories When Opening Files is selected in the system policies, you cannot change directories or drives to locate a file to select. ▲

#### 3. Choose OK.

If the configuration file has a password, a prompt asks for the password. Type the password in the text box and choose OK. (You are allowed three attempts.)

The software is set up as specified by the configuration you opened.

#### Note for DS systems

Access to standard menu items is controlled by the Security Administration software, regardless of the settings in the opened configuration. ▲

## Saving a configuration

Use Save Configuration As in the File menu to save the current software configuration in a configuration file on a disk. If you do not have the DS option, the configuration determines the settings of the options in the Options dialog box and which features appear in the OMNIC menus and the toolbar. If you have the DS option, the configuration determines the settings of the options in the Options dialog box, except for those in the Directories box on the File tab, and which command buttons are active in the toolbar. (The default directories, which commands are enabled in the menus, and which toolbar buttons are active are determined by the Security Administration software.)

See “Customizing the OMNIC menus” and “Customizing a toolbar” in the “Edit” chapter for details on creating a configuration that sets up the software according to your preferences.

If you do not have the DS option, you can assign a password to your configuration file within OMNIC to prevent unauthorized users from changing and then saving your configuration with the changes.

**Note** Whenever you are asked to enter an OMNIC password, you are allowed three attempts to enter the correct password before the software ends the procedure. ▲

You can open the saved configuration later by using Open Configuration in the File menu. This makes it easy to set up the software without having to set individual parameters. See “Opening a configuration” for details.

Depending on whether the log-in feature is on or off, the Set As Default Configuration option in the Save Configuration dialog box lets you specify that the configuration be associated with your user name or be used as the default configuration. (This does not apply to systems with the DS option. Those systems use the Security Administration software to assign configurations.)

To prevent unauthorized users from saving a changed configuration, we recommend hiding the Save Configuration As command (using Edit Menu in the Edit menu). If you have the DS option, use the access control features of Security Administration to prevent specified users from using the command. You can also use the Default Configuration system policy to specify a configuration directory for specified users.

## ■ **How to** ➡ Save a configuration

This procedure varies depending on whether you have the DS option.

*Follow these steps if you do not have the DS option:*

### **1. Choose Save Configuration As from the File menu.**

The Save Configuration As dialog box appears.

### **2. Type a filename in the File Name text box.**

Use the extension .CON. To overwrite an existing file, click the filename in the list of configuration files.

### **3. Turn the Set As Default Configuration option on or off as desired.**

- If the log-in feature is currently on, turning on the Set As Default Configuration option associates the configuration with your user name (replacing the currently associated configuration) so that it is used the next time you log in.
- If the log-in feature is currently off, turning on this option designates the configuration as the new default configuration so that it is used the next time OMNIC is started with the log-in feature turned off.

### **4. If you want to assign a password to the file or overwrite a password-protected file and assign a new password, choose Password.**

- If you are entering a password for a new file (that has a new filename) or for an existing file that does not have a password, a dialog box asks for the password. Type a password in the text box and then choose OK. A dialog box asks you to confirm the password. Type the password in the text box and then choose OK. A message informs you that the password has been assigned. Choose OK. The procedure is finished.

- If you are overwriting a password-protected file and assigning a new password, a dialog box asks for the current password. Type the file's current password in the text box and then choose OK. A dialog box asks for the new password. Type the new password in the text box and then choose OK. A dialog box asks you to confirm the password. Type the new password in the text box and then choose OK. A message verifies that the new password has been assigned. Choose OK.

**5. If you want the configuration saved so that it can be opened later but not changed and saved with the changes, turn on the Read Only check box near the lower-left corner of the dialog box.**

**6. Choose OK.**

If you specified a filename that is in use by a password-protected file and you did not use the Password button to change the password, a dialog box asks you to enter the password. Type the password in the text box and then choose OK.

*Follow these steps if you have the DS option:*

**Note** You may be prompted to digitally sign a file; follow the instructions that appear on the screen. If you are not prompted but want to sign the file, turn on Use Digital Signature in the Save Configuration dialog box. ▲

**1. Choose Save Configuration As from the File menu.**

The Save Configuration As dialog box appears.

**2. Type a filename in the File Name text box.**

Type a filename in the File Name text box. To overwrite an existing file, click the filename in the list of configuration files. (You cannot overwrite a file if Prevent Overwriting Of Files is selected in the system policies.)



3. **If you want the configuration saved so that it can be opened later but not changed and saved with the changes, turn on the Read Only check box near the lower-left corner of the dialog box.**
4. **Choose OK.**

## Logging into OMNIC as a different user

Use Log In in the File menu to log in as a user of OMNIC. When you log in, OMNIC loads the configuration that is associated with your user name. This sets up the menus, the toolbar and the software options according to your preferences.

**Note for DS systems** This command is not available in your software. Log onto Windows using features provided by the operating system. ▲

**Note** You can add names to the list of users by using Add User Name in the File menu. (That command is not available on systems that include the DS option.) You can then set up the software and save your settings in a configuration. The next time you log in, that file will be used. See “Adding a user name” for details. ▲

**Note** To turn the log-in feature on or off after installing the software, use Enable OMNIC Log-In in the File menu. See “Turning OMNIC log-in on or off” for details. ▲

### ■ *How to* ➡

Log into OMNIC as a different user

1. **Choose Log In from the File menu.**

**Note for DS systems** The Log In command is not available in your software. ▲

A dialog box appears.

2. **Type a user name (normally your name) in the text box.**
3. **Choose OK.**

If you entered a name that is not recognized by OMNIC’s log-in feature, a message informs you. Choose OK and then enter a valid name.

If the configuration file associated with the entered user name has a password, a prompt asks for the password. Type the correct password in the text box and choose OK. (If you fail to enter the correct password after three attempts, OMNIC runs but only the Log In and Exit commands in the File menu are available.)

The software is set up as specified by the configuration file associated with the user name.

**Note** If you specified a default experiment for your user name (either when you saved an experiment or added your user name), that experiment is selected automatically. ▲

## Adding a user name

Use Add User Name in the File menu to add your name as a user of OMNIC. This lets you log into OMNIC later and automatically load the configuration file associated with your name to set up the software according to your preferences. When you add your name, the current configuration file is associated with your name.

**Note for DS systems** This command is not available in your software. You can add users to user groups with features provided by Windows Vista™ or Windows XP. ▲

**Note** To turn the log-in feature on or off after installing the software, use Enable OMNIC Log-In in the File menu. See “Turning OMNIC log-in on or off” for details. ▲

### — *How to* ➔

Add a user name

- 1. Set up the software configuration as desired and save it using Save Configuration As in the File menu, or use Open Configuration in the File menu to open the configuration that you want to associate with your name.**

To set up the current configuration, use Options, Edit Menu and Edit Toolbar in the Edit menu (the “Edit” chapter explains how to use these commands). If you save the configuration, assign a password to it if you don’t want other users to be able to use it or change it. See “Saving a configuration” for details.

**2. Choose Add User Name from the File menu.**

The Add User Name dialog box appears.

**Note** If Add User Name is not available in the File menu, use Enable OMNIC Log-In in the File menu to enable it. See “Turning OMNIC log-in on or off” for details. ▲

**Note for DS systems** The Add User Name command is not available in your software. ▲

**3. Type a new user name in the text box and then choose OK.**

The Select Configuration File dialog box lists the available configuration files (with the extension .CON). The provided example configuration files are in the Param directory within the OMNIC directory.

**4. Type the name of the file you want to associate with the new user name, or locate a file and select it by clicking its filename.**

**5. Choose OK. The Select Experiment File dialog box lists the available experiment files (with the extension .EXP).**

**6. Type the name of the file you want to use, or locate a file and select it by clicking its filename.**

**7. Choose OK.**

**Note** If you want to make the Add User Name command unavailable in this configuration, add your user name and then use Edit Menu to make the command disabled or hidden and save the change using the Save button in the Edit Menu dialog box. ▲

## Turning OMNIC log-in on or off

Use Enable OMNIC Log-In in the File menu to turn OMNIC’s log-in feature on or off. If you start OMNIC when the feature is on, the software asks you to enter a user name. If the configuration associated with the entered name has a password, or if your system includes the DS option, you are asked to enter a password as well.

If you start OMNIC when the log-in feature is off, you are not asked to enter a name or password.

See “Logging into OMNIC” for more information about logging in.

**Note** The Enable OMNIC Log-In command may not be available if the system manager has set up a controlled system. ▲

**Note for DS systems** This command is not available in your software. When you start OMNIC DS, the Windows software prompts you to log on. ▲

### — *How to* ➔

Turn OMNIC log-in on or off

#### 1. Choose Enable OMNIC Log-In from the File menu.

A message asks if you’re sure you want to turn on the log-in feature.

#### 2. Choose Yes.

A check mark appears next to the command name in the menu to indicate that the command is on. When the command is on, you are asked to enter a user name (and password if required by the configuration associated with the name or if your system includes the DS option) whenever you start OMNIC.

To turn the command off, choose Enable OMNIC Log-In from the File menu when the check mark is present. The check mark is removed.

**Note for DS systems** This command is not available in your software. When you start OMNIC DS, the Windows software prompts you to log on. ▲

## Opening or closing a log

Use Open Log in the File menu to open or create a log file in which to automatically record your data collection and processing operations. A log is a list of data collection and processing operations that have been performed, along with the results of the operations, during the time that the log was open. Examples of these operations include collecting a spectrum, measuring the area under a peak with the peak area tool, and correcting a baseline.

The log is displayed in the log window (see the example below), which appears after you select and open a log file.

You can edit the information in the log and print its contents on paper.

```

Log File - C:\OMNIC\EXAMPLE.LOG
Mon Jun 29 09:44:29 1998
BASELINE CORRECT(Linear):
  Spectrum: Example
  Baseline points list:
    X: 2748.109 Y: -0.006
    X: 2813.858 Y: -0.006
    X: 2870.125 Y: 0.034
    X: 2993.405 Y: 0.014
    X: 3045.246 Y: -0.045
    X: 3117.950 Y: -0.222
    X: 3190.653 Y: -0.006
    X: 3207.091 Y: -0.006

Mon Jun 29 09:45:08 1998
FIND PEAKS:
  Spectrum: Polystyrene measured as a film
  Region: 3371.67 2681.55
  Absolute threshold: 1.253
  Sensitivity: 50
  Peak list:
    Position: 2923.66 Intensity: 2.459
    Position: 3025.69 Intensity: 2.334
  
```

**Note** If Save Log As RTF File is turned on in the File options (available through Options in the Edit menu), you can copy a spectrum in a spectral window and paste it into a log. To delete a pasted spectrum, click it to select it and then press the Delete key. If you paste a spectrum at the end of a log and the spectrum's image is larger than the displayed log window, you can select the image and then use the right arrow key on the keyboard to go to the end of the log. ▲

The Open Log command toggles between Open Log and Close Log. If your work is currently being recorded in a log, this command appears in the File menu as Close Log. When you choose Close Log, the recording of your work is stopped, the log window is removed from the screen and the command name changes to Open Log. To resume recording your work in a log, choose Open Log; the command name will change to Close Log after you open a log file.

You can save the log as a text file or rich text format file on the hard disk. See "Saving a log as a rich text format (RTF) file" in the "Edit" chapter for details.

You can create and use different log files to keep separate records of your work. The log you use will be displayed in a window named for the file that contains the log and the path to the file.

**— How to ➡**

Open or close a log

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

A dialog box lists files of the Log Files (\*.LOG) file type.

**2. To use an existing log, type the name of the log file you want to open or locate a file and select it by clicking its filename.**

You can change directories or drives to locate the file you want to use. Log files normally use the extension .LOG.

**Note for DS systems**

If Prevent Changing Directories When Saving Files is selected in the system policies, you cannot change directories or drives to locate a file to open. ▲

**3. Choose OK to start logging in the file you specified.**

The log window appears. The title bar of the window shows the pathname of the log file you have opened. If the log contains information from previous operations, the information appears in the window as text. You can use the scroll bar at the right side of the window to bring logged information into view.

As you perform operations, information is added to the window at the end of any existing text.

To minimize the log window, click its Minimize button. The log will continue to record information.

**4. To stop logging, choose Close Log from the File Menu.**

The log window is removed from the screen and the logged information is saved in the log file automatically.

**Note**

If a spectrum has been pasted into the log window, you must turn on Save Log As RTF File in the File options (available through Options in the Edit menu) if you want the image saved with the log. ▲

## Printing

Use Print in the File menu to print spectra in a spectral window, the contents of the log window, or information contained on a tab of Library Manager. When you print spectra contained in a spectral window, they are printed in the same order as they appear on the screen. If you are displaying a spectral region, that region is printed.

To specify margin sizes and other printing options, use Options in the Edit menu to set the Print options.

**Note** To print a report, use Preview/Print Report in the Report menu. See “Previewing or printing a report” in the “Report” chapter for details. ▲

### ■ *How to* ➔

Print information

#### 1. Use Options in the Edit menu to set the Print options as desired.

The changes you make to the Print options will take effect when you print a spectral window (or a report using Preview/Print Report) or when you next add an image to the log window. The display of spectra in a spectral window is not affected by the Print options. See “Print options” in the “Edit” menu for complete information on using the Print options.

#### 2. Display the items you want to print.

If you are printing spectra, arrange them in the spectral window exactly as you want them to appear on paper.

If you are printing spectra in a spectral window, make sure the window is selected when you are finished arranging the spectra.

If you are printing a log, select the log window by clicking anywhere inside it.

If you want to print information contained on a tab of Library Manager, display that tab. See “Managing libraries” in the “Analyze” chapter for information on displaying tabs of Library Manager.

**3. Make sure the printer is turned on and ready.**

**Note** If you are printing a log, it will be printed on the default printer, regardless of which printer is selected in the Print Setup dialog box. ▲

**4. Choose Print from the File menu.**

The Print dialog box appears. It lets you specify items such as the number of pages to print. (See your Windows documentation for details on using this dialog box.)

**5. Set the parameters as desired and then choose OK or Print.**

## Setting up the printer

Use Printer Setup in the File menu to specify a printer and set the page orientation and other print parameters before you print images or information on paper. See “Printing” for more information.

### — *How to* ➔

Set up the printer

**1. Choose Printer Setup from the File menu.**

The Print Setup dialog box appears.

**2. Select the printer from the list box.**

You can also specify portrait or landscape page orientation.

**Note** If you change the orientation using Printer Setup, the Orientation option in the Print options (available through Options in the Edit menu) will be reset to the new orientation. The page orientation setting in Windows Control Panel or in the printer setup dialog box for other applications is not affected by the setting you make here. See “Specifying how to print spectra” in the “Edit” chapter for more information on the Orientation option. ▲

**Note** If you are printing a log, it will be printed on the default printer, regardless of which printer is selected in the Print Setup dialog box. ▲



3. **If you want to set the printer parameters, choose Properties. If you don't want to set the parameters, choose OK.**

If you choose Properties, a dialog box shows the current settings of the printer parameters. This dialog box varies in appearance depending on your printer. See the documentation that came with your printer for information on setting the printer parameters. After you set the printer parameters, choose OK to close the dialog box, and then choose OK to close the Print Setup dialog box.

## Deleting files

Use Delete Files in the File menu to delete spectral data files, configuration files, experiment files, log files and other kinds of files and place them in the Windows Recycle Bin.

### — *How to* ➔

Delete files

1. **Choose Delete Files from the File menu.**

The Delete Files dialog box lists files of the Spectra (\*.SPA) file type. You can list files of other types by selecting a type from the List Files Of Type drop-down list box.

2. **Type the name of the file you want to delete, or locate and select one or more files.**

To select one file, click its filename. To select more than one file, hold down the Control key and click the desired filenames. You can change directories or drives to locate the files.

### **Note for DS systems**

If Prevent Changing Directories When Saving Files is selected in the system policies, you cannot change directories or drives to locate a file to open. ▲

If you select a file that contains just one spectrum, the spectrum's title appears in the Spectrum Title box. If you select more than one file, the last selected spectrum's title appears.

3. **Choose OK.**

The files are deleted from the hard disk.

## Exiting OMNIC

Use Exit in the File menu to leave OMNIC. Depending on the amount of memory your computer has, you may need to exit OMNIC before you can open other applications, such as word processing and graphics programs. You should also exit before shutting off your computer.

### — *How to* ➔

Exit OMNIC

#### **Choose Exit from the File menu.**

Depending on the settings of the software options and whether you have changed any spectral data, a message may appear asking you whether to save the data before closing. Choose Yes to save the data, No to close without saving, or Cancel to keep OMNIC open.

# Edit

The Edit menu includes commands that let you perform these operations:

To do this...	Use this command...
Reverse the effects of operations.	Undo
Remove items from a window.	Cut
Copy items in a window.	Copy
Paste items into a window.	Paste
Place a duplicate of a spectrum into a spectral window.	Paste Image
Delete spectra from a spectral window.	Clear
Select all the spectra in a spectral window.	Select All
Delete labels and other annotation.	Delete Annotation
Customize the software by setting options that affect its operation.	Options
Customize the OMNIC menus.	Edit Menu
Create custom toolbars containing buttons for initiating menu commands.	Edit Toolbar

## Undoing operations

Undo in the Edit menu lets you reverse the effects of various operations.

For example, if you have just replaced a region of a spectrum with a straight line using Straight Line in the Process menu, you can restore the original data by choosing Undo. If you choose Undo again, the changed spectrum is redisplayed and you can continue where you left off.

The Undo command is available only if you are allowed to undo the operation you just performed. You cannot undo operations that were performed simultaneously on multiple spectra using Process menu commands.

**— How to ➔** Undo the effects of a command or operation

**Choose Undo from the Edit menu.**

To restore the changes you just reversed, choose Undo again.

## Cutting items

Cut in the Edit menu removes the selected spectra, images or text from the active window and places the cut items onto the Windows Clipboard (replacing the previous contents, if any exist). After you cut an item, you can use Paste to place a copy of the item in another location. (The location can be in OMNIC or in another appropriate Windows application such as a spreadsheet, word processing or graphics program.) See “Pasting an item” for more information on using Paste.

When you cut a displayed stacked spectrum, the displayed spectra below it move up one pane so that the pane which contained the cut spectrum is filled.

If any spectra remain in the spectral window after you cut the selected spectra, one of the remaining spectra will be selected automatically.

**Note** When you cut an item, OMNIC places it on the Clipboard in two formats: bitmap (BMP) and Windows metafile (WMF). When you use an application to paste the item from the Clipboard, the application selects the appropriate format; for example, Microsoft® Word selects WMF and Microsoft Write selects BMP. Bitmaps don’t resize well. Metafiles produced by OMNIC can be resized with better results, but they take longer to produce. ▲

**— How to ➔** Cut items

### 1. Select the items.

To select text, use standard Windows editing techniques such as double-clicking or dragging.

### 2. Choose Cut from the Edit menu.

The selected items are removed from the window and stored on the Windows Clipboard.

## Copying items

Copy in the Edit menu places a duplicate of the selected spectra, text or images onto the Windows Clipboard (replacing the previous contents, if any). After you copy an item, you can use Paste to paste a copy of the item into another location. (The location can be in OMNIC or in another appropriate Windows application such as a spreadsheet, word processing or graphics program.) See “Pasting an item” for more information.

**Note** When you copy an item, OMNIC places it on the Clipboard in two formats: bitmap (BMP) and Windows metafile (WMF). When you use an application to paste the item from the Clipboard, the application selects the appropriate format; for example, Microsoft Word selects WMF and Microsoft Write selects BMP. Bitmaps don't resize well. Metafiles produced by OMNIC can be resized with better results, but they take longer to produce. ▲

### — *How to* ➔

Copy items

#### 1. **Select the items.**

To select text, use standard Windows editing techniques such as double-clicking or dragging.

#### 2. **Choose Copy from the Edit menu.**

The items are copied onto the Windows Clipboard.

## Pasting items

After you cut or copy spectra, text or images, a duplicate of the cut or copied items is on the Windows Clipboard. You can use Paste in the Edit menu to place a copy of the items in the location you specify. See “Cutting items” and “Copying items” for information on using the Cut and Copy commands.

If you paste a spectrum into a spectral window, both the spectral data and their graphical representation are “passed” into the window and you can begin processing and manipulating the spectrum. The pasted spectrum is initially an exact copy of the spectrum that was cut or copied to the Clipboard.

You can continue to paste copies until you cut or copy another selected item.

**Note** If you paste a spectrum into the log window, turn on Save Log As RTF File in the File options (available through Options in the Edit menu) if you want the image saved with the log. See “Saving a log as a rich text format (RTF) file” for details. ▲

### — *How to* ➔

Paste items from the Clipboard

1. **Click the spectral window or location where you want to paste the items.**
2. **Choose Paste from the Edit menu.**

The contents of the Windows Clipboard are placed in the location you clicked. If you are pasting a spectrum into a spectral window, the spectrum will be selected and can immediately be used in other operations. If you are pasting text, the text starts at the insertion point.

## Pasting duplicate images of spectra

After you copy a spectrum or spectra to the Windows Clipboard, you can use Paste Image in the Edit menu to place a duplicate image of the spectrum or spectra into another spectral window. The original spectrum and the duplicate are “linked” (they have one common set of data) so that any change you make to one is simultaneously made to the other. This lets you compare the duplicate with other spectra as you make changes to the original. See “Copying items” for information on using the Copy command to copy spectra to the Clipboard.

### — *How to* ➔

Paste duplicate images of spectra

1. **If you have not already copied the spectra, use Copy to copy them onto the Windows Clipboard now.**

Be sure to select and copy all of the spectra at the same time.

2. **Create a new spectral window or select an existing window into which to paste the images of the spectra.**

If you want to paste the image into a new spectral window, use New Window in the Window menu to create the window. See “Creating a new spectral window” in the “Window” chapter.

### 3. Choose Paste Image from the Edit menu.

## Deleting spectra

Use Clear in the Edit menu to delete all the selected spectra and spectrum images from the active spectral window. Unlike cutting items with Cut, clearing an item does not place a copy of it onto the Windows Clipboard.

When you clear a displayed stacked spectrum, the spectra below it move up one pane so that the pane which contained the cleared spectrum is filled.

If any spectra remain in the window after you clear the selected spectra, one of the remaining spectra is selected automatically.

### — How to ➡

Delete spectra

1. **Select the spectra (or images create with Paste Image) you want to clear.**
2. **Choose Clear from the Edit menu.**

## Selecting all the spectra in a spectral window

Use Select All in the Edit menu to select all the spectra in the active spectral window except any hidden spectra. This is useful when you want to perform an operation on more than one spectrum at the same time; for example, clearing spectra, adding spectra or saving spectra as a group. Locked spectra are selected along with the other spectra.

### — How to ➡

Select all the spectra in a spectral window

1. **Select the spectral window.**

If only one spectral window currently exists, that is the selected window.

2. **Choose Select All from the Edit menu.**

All the spectra that are not hidden become selected.

## Deleting annotations

Use Delete Annotation in the Edit menu to delete the selected annotations from the active spectral window. The deleted annotations are not placed on the Windows Clipboard.

**Note** You can also delete a label by using the annotation tool. See “Annotation tool” in the “About the Display” chapter for details. ▲

### — *How to* ➔

Delete annotations

#### 1. **Select the annotations by drawing a box around them with the selection tool.**

Be sure to completely enclose the annotation text with the box. If the text is not completely enclosed, it will not be selected. There is no need to enclose the lines that connect the annotations to the spectrum. See “Selection tool” in the “About the Display” chapter for complete information on using the selection tool.

#### 2. **Choose Delete Annotation from the Edit menu.**

You can also delete the annotation by holding down the Control key and clicking inside the box you drew to select the annotation.

**Note** You can also delete the annotations by holding down the Control key and clicking inside the box you drew to select the annotations. ▲

## Customizing OMNIC by setting options

Use Options in the Edit menu to customize OMNIC for the way you prefer to use the software. You can set options that affect how spectra are collected, displayed, processed, saved and printed. These options settings are saved in a configuration file. A lab manager can create and save a configuration file for each user of the software so that only the appropriate features are available when that configuration is in use.

**Note** The options you set using Options are different from the experiment parameters you set using Experiment Setup in the Collect menu. The options are normally set according to how you or other users prefer to use the software. The experiment parameters, on the other hand, are normally set according to the type of data being collected or analyzed. ▲



The Options dialog box displays any one of several sets of options: File, View, Print, Collect, Process and Window. (If you have OMNIC Atlas™ 7.0 or greater, other tabs also appear. See the *OMNIC Atlas User's Guide* for more information.) Each set is contained on a tab whose name is always visible at the top of the dialog box. To display a set of options, click the appropriate tab. The options are brought to the front.

After you have set the options, you can save them in a configuration file by using Save Configuration As in the File menu. See “Saving a configuration” in the “File” chapter for details.

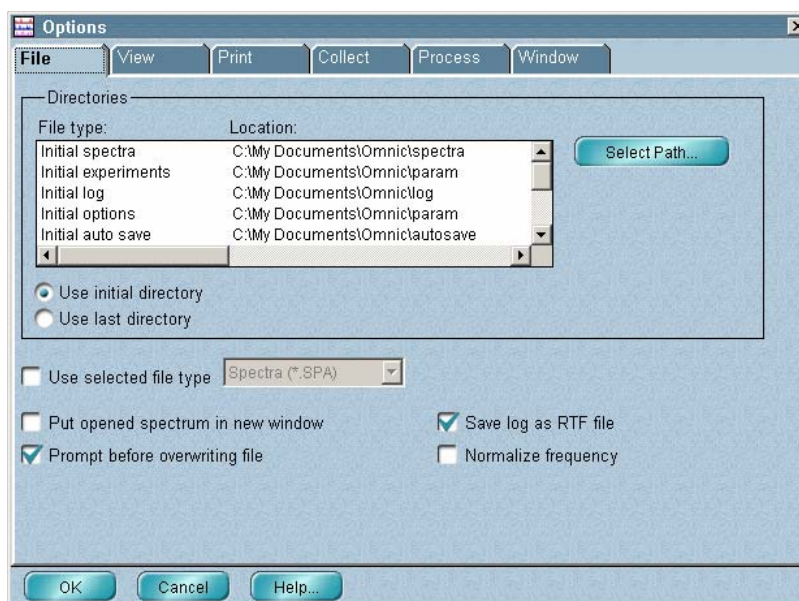
To use the options you have saved in a configuration, use Open Configuration in the File menu. When you open the file, OMNIC is set up according to your preferences. See “Opening a configuration” in the “File” chapter for more information.

To change the settings in your options, open your configuration and then make the desired changes. To save the settings, use Save Configuration As in the File menu.

The following sections describe the six sets of options.

## File options

The File options appear when you click the File tab.



The following table shows what you can specify with each option.

To specify or do this...	Use this feature...
The default directories for operations.	Directories
The default file format for opening and saving spectra.	Use Selected File Type
Place opened spectra into new spectral windows.	Put Opened Spectrum In New Window
Display a warning before overwriting a file.	Prompt Before Overwriting File
Save logs as rich text format (RTF) files.	Save Log As RTF File
Normalize the frequency automatically when the file is opened.	Normalize Frequency

The next sections explain how to set these options.

## Specifying directories

### Use initial directory

The Directories box in the File options (available through Options in the Edit menu) shows the current default directory locations (paths) for a variety of operations. The file types for these items are listed in the File Type column of the list box, and the corresponding directories are listed in the Location column. These directories will be used if Use Initial Directory is selected. For example, when you use the Open command to open a spectrum, the Open dialog box will initially show the spectral data files contained in the default directory. Similarly, when you use the Save As command to save a spectrum, the Save As dialog box will be set up to save the spectrum in this default directory.

### Use last directory

If you want open and save operations to use the directory that was used last instead of the specified default directories, select Use Last Directory.

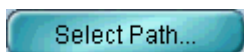
### Note

The Initial User Library directory is used regardless of whether Use Initial Directory or Use Last Directory is selected. ▲

The file types described in the following table are available.

**Note for DS systems**

The Initial Spectra, Initial Experiments, Initial Quant, Initial Macro, Initial User Library, Initial Report and Initial Auto Save file types do not appear in the Directories box. Use the system policies in the Security Administration program to specify default directories for operations involving these file types. ▲

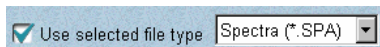


To specify a different default directory location for a file type, select the file type in the list box and then choose Select Path, or just double-click the file type in the list. In the dialog box that appears type the path to the desired directory in the text box and then choose OK. The new path then appears in the Location column.

File Type	Description
Initial Spectra	Spectral data files opened using Open in the File menu or saved using Save As in the File menu. (This file type also includes spectra saved using Save if the spectrum has not been saved before. In this case, the Save As dialog box appears when you save the spectrum.)
Initial Experiments	Experiment files selected using the Experiment drop-down list box or the Open button in the Experiment Setup dialog box, and experiment files saved using the Save As button in the dialog box.
Initial Log	Log files opened using Open Log in the File menu.
Initial Auto Save	Spectral data files saved automatically when the Save Automatically option is turned on in the Experiment Setup dialog box.
Initial Macro	Macro files opened or saved using the optional OMNIC Macros\Basic software. Macros let you automatically perform sequences of operations. See your Macros\Basic documentation for details.
Initial User Library	Library files used by Library Setup and Library Manager in the Analyze menu. The directory for this file type is used as the default directory for storing new libraries you create with the Create Library button in Library Manager.
Initial Quant	Quantitative analysis methods opened using Quant Setup. See “Selecting a quant method” in the “Analyze” chapter for details.

File Type	Description
Initial Report	Report template files selected, edited or created with Template in the Report menu and reports previewed or printed with Preview/Print Report in the Report menu.

### Specifying a file type for opening and saving spectra



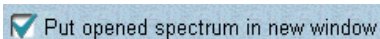
To specify a file type to be used whenever you open or save spectra using Open or Save As in the File menu, turn on Use Selected File Type and select the desired file type from the drop-down list box. The selected file type will also be used when you save a spectrum for the first time using the Save command in the File menu.

The DOS extensions used for each file type are shown in the following table.

File Type	Extension for Opening	Extension for Saving
Spectra (the default)	.SPA	.SPA
JCAMP-DX	.JDX	.JDX
PCIR	.IRD	.IRD
Nicolet SX/DX	.NIC or .SPC	.NIC
GRAMS/386	.SPC or .GLD	.SPC
Mattson	.ABS	.ABS
Spectacle	.IRS	.IRS

If Use Selected File Type is off, the file type used when you open or save a spectrum will be the same type that was last used for that operation.

### Placing opened spectra into new spectral windows



If you want spectra you open to always be placed into new spectral windows, turn on Put Opened Spectrum In New Window. If you open more than one spectrum at a time, each will be placed into a separate window. If you turn this option off, opened spectra will be placed into the active spectral window, or into a new spectral window if no spectral window exists. When an opened spectrum or spectra are placed into a new spectral window, a default title is automatically given to the window.

### Displaying a warning before overwriting a file

Prompt before overwriting file

Turn on Prompt Before Overwriting File if you want OMNIC to warn you before overwriting a spectral data file or configuration file with the same name. The warning will be displayed as needed when you use Save As or Save Configuration As in the File menu. If the warning appears, you will be allowed to overwrite the file or use a different filename.

#### Note

This option applies to Mattson spectral data files only if they have the extension .ABS (Absorbance). You will not be warned before overwriting a Mattson file having any of the following extensions: .RAS (Transmission and %T), .IGM (Interferogram), .SBM (Single Beam) and .DRT (Kubelka-Munk). ▲

We recommend that you keep this option on to prevent accidental overwriting of valuable files.

### Saving a log as a rich text format (RTF) file

Save log as RTF file

Turn on Save Log As RTF File if you want the log to be saved as a rich text format (RTF) file when you close the log window or exit OMNIC. Rich text format includes more text formatting than regular text format. This formatting may be desirable if you open the file using a word processing or other program.

If the option is off, the log will be saved as a regular text file. If you want spectra contained in the log window to be saved with the log, turn this option on; these graphical images can be saved only in rich text format.

### Normalizing the frequency automatically

Normalize frequency

The Normalize Frequency option lets you specify whether the laser frequency of spectra you open is automatically normalized. Normalizing the frequency changes the locations of the spectral data points to standard positions; that is, the positions they would be at if they had been collected using a spectrometer with a reference laser frequency of 15,798.0 wavenumbers. This results in better correspondence of data collected using spectrometers with slightly different laser frequencies.

Normalize the spectra of standards and unknown samples if you develop or use a quant method on more than one spectrometer. You should also normalize noncalibrated spectra; that is, JCAMP-DX spectra, spectra from CSV (comma-separated values) text files, and spectra collected using dispersive instruments.

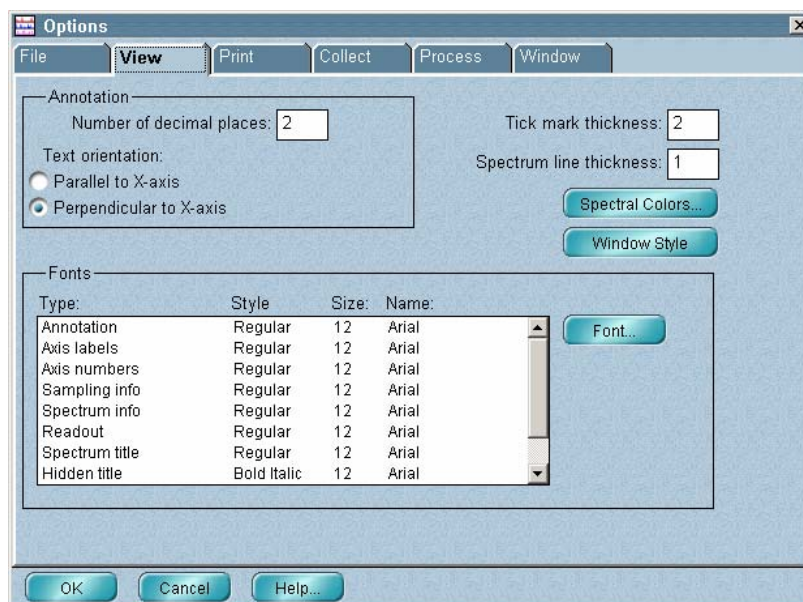
The frequency is normalized only if it is not equal to the reference frequency and the difference between the two is less than 20 wavenumbers.

**Notice** Normalizing the frequency of spectra guarantees that data points occur at the same frequency positions. This lets you move data between spectrometers without the problems associated with inconsistent data point positioning. However, if you plan to analyze sample spectra using previously calibrated quant methods developed with a version of OMNIC earlier than 3.0, *do not normalize the frequency of the sample spectra*. If you normalize your sample spectra and attempt to use a calibrated method whose standards were not normalized, the data will not match and the analysis will fail. ▲

**Note** You can use Normalize Frequency in the Collect options to specify whether to normalize the frequency automatically when you collect a spectrum. See “Collect options” for details. You can use Normalize Frequency in the Process menu to normalize the laser frequency of a spectrum already displayed in a spectral window. See “Normalizing the frequency of a spectrum” in the “Process” chapter for details. ▲

When you normalize the frequency of a spectrum, a record of the operation is made in the “DATA PROCESSING HISTORY” section of the Collection And Processing Information window.

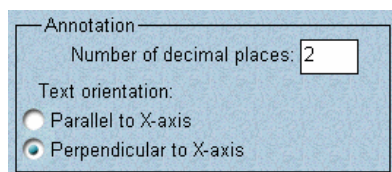
**View options** The View options appear when you click the View tab.



They let you specify how to display items in spectral windows. The table below shows what you can specify with each option.

To specify this...	Use this feature...
The number of decimal places in annotations.	Number Of Decimal Places
The orientation of annotation text.	Text Orientation
The thickness of tick marks of displayed axes.	Tick Mark Thickness
The line thickness for displaying spectra.	Spectrum Line Thickness
The colors for displaying spectra and other features.	Spectral Colors
The style of appearance for windows and dialog boxes in OMNIC.	Window Style
The fonts for displaying text.	Fonts

### Specifying how to display annotations



Specify the number of decimal places (digits to the right of the decimal point) you want used for numbers that appear in newly created annotations and peak labels by typing a number in the Number Of Decimal Places text box. The maximum number of places is 5. Existing annotations and labels are not affected by changes to Number Of Decimal Places.

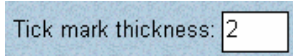
The options in the Annotation box deal with the display of peak labels and other annotations.

Use the Text Orientation option buttons to specify how to display existing and newly created peak labels and other annotation text.

If you want the text to be parallel to the X-axis, select Parallel To X-Axis.

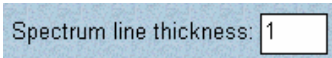
If you want the text to be perpendicular to the X-axis, select Perpendicular To X-Axis.

### Specifying the thickness of tick marks



To specify the thickness of the tick marks displayed along the axes, type the desired value in the Tick Mark Thickness text box. The thickness is measured in pixels. The allowed values are 1 through 6.

### Specifying the spectrum line thickness

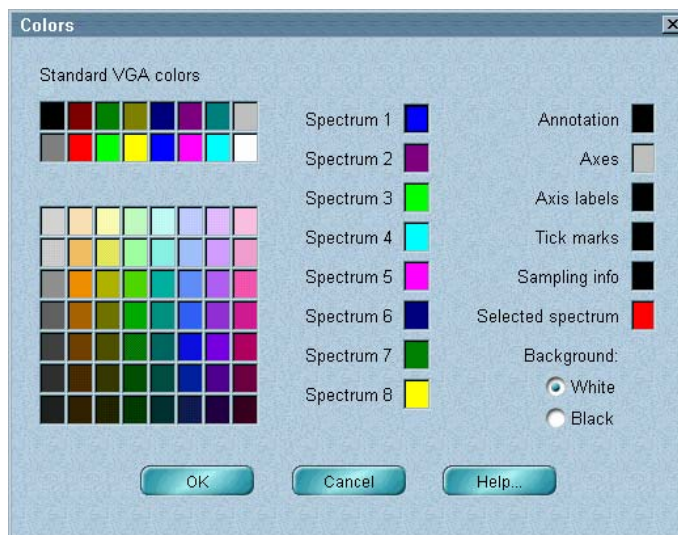


Specify the thickness of the lines used to display spectra by typing the desired value in the Spectrum Line Thickness text box. The thickness is measured in pixels. The allowed values are 1 through 10. A thickness of 1 gives the finest line and therefore the most detailed image.

### Specifying colors for spectra and other features



The Spectral Colors button lets you specify the colors to use for displaying spectra, annotations, axis labels, tick marks and sampling information in spectral windows. When you choose Spectral Colors, the Colors dialog box appears.



In the upper-left corner of the dialog box are two rows of standard colors that can be displayed on VGA monitors.

If your system has the needed hardware for displaying 256-color images, an array of other colors appears below the standard VGA colors.

To the right of the color array are shown the eight currently selected colors for displaying non-selected spectra. These colors are used in the order shown as spectra are added to a spectral window. After a spectrum is displayed using the last color, the assignment of colors starts again with the first color.



To change one of the eight selected display colors, click the box containing the display color you want to change and then click the desired color in the VGA colors or in the array of other colors. The new color appears in the box. The colors you select here will be available in the Display Setup dialog box for changing the color of spectra. See “Selecting a color for the currently selected spectra” in the “View” chapter for more information.

At the far right of the dialog box are the currently selected colors for displaying annotation text, axis label text, sampling information and selected spectra. You can specify colors for displaying these items in the same way as explained above for selecting colors for displaying spectra. If you specify white or black for displaying annotations or sampling information, the actual color used will be changed when necessary to make the text visible against the background. The color specified for annotations will also be used to display the titles of stacked spectra in their panes.

**Note** If the color you specify for selected spectra is already assigned to one or more non-selected spectra, the color previously assigned to selected spectra will be assigned to those non-selected spectra. ▲

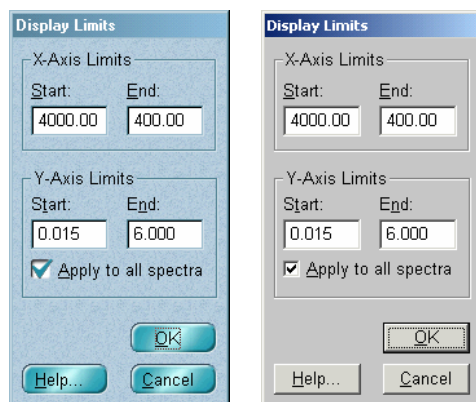
To select a background color for spectral window panes, set Background to White or Black by clicking the appropriate option button. If you specify a black background, some features (for example, the spectral cursor will be displayed in white to make the features visible against the background. If you select Black, make sure the colors you specify for displaying spectra will be visible on a black background.

When you have finished specifying colors, choose OK to return to the View options.

## Selecting a style for windows and dialog boxes



The Window Style button lets you customize the appearance of the windows and dialog boxes in OMNIC. Several window styles are available. Here is an example showing a dialog box displayed using two of the available styles:



Each time you click the Window Style button, a different style appears. Click the button until the desired style is displayed.

**Note** This feature has no effect if your system is set to display 256 or fewer colors. ▲

**Note** Be sure to save the configuration so that your window style will be in effect whenever you use OMNIC with that configuration. ▲

## Specifying fonts for displayed text

The Fonts list box lets you specify which fonts, styles and sizes to use when displaying various types of text. The Style column in the list box indicates the font style used for each text type. Examples of styles are Regular, Italic, Bold and Bold Italic. The Size column shows the current font size in points. The Name column shows the current font name.

Each text type is listed in the Type column of the list box and is described in the following table.



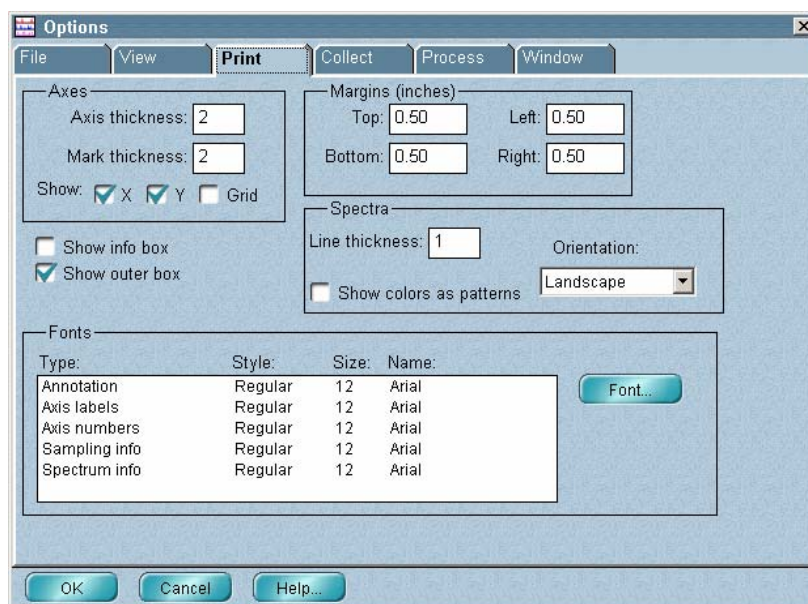
To change the font or font size for a type of text, select the text type in the list and then click the Font button, or just double-click the text type in the list. The Font dialog box appears. Select a font from the Font list box, a style from the Font Style list box and a size from the Size list box. A sample of the currently specified text is shown in the Sample box. When you have finished specifying the text, choose OK. The new text specifications appear in the Fonts list box.

Type	Description
Annotation	A label or other text created using the palette tools or Find Peaks (often used to state the frequency location or significance of a spectral feature), and the titles of spectra displayed by Display Overlaid Titles available through Options in the Edit menu. See “Annotation tool” in the “About the Display” chapter, “Finding peaks” in the “Analyze” chapter or “Spectral View” in the “Edit” chapter for details.
Axis Labels	Axis labels showing the units of the X-axis and Y-axis in a spectral window. To ensure that the axis labels are displayed correctly, use only TrueType® fonts.
Axis Numbers	Numbers that appear along the X-axis and Y-axis in a spectral window.
Sampling Info	Information displayed within a spectrum’s pane when the Sampling Information option is turned on and one or more items are selected in the Sampling Information box in the Display Setup dialog box. See “Displaying sampling information” in the “View” chapter for more information.
Dialog Boxes	Information contained in the Collection And Processing Information window. (You can display this information by double-clicking a spectrum title in the title box.) See “Collection and processing information” in the “About the Display” chapter for details.
Readout	X and Y values and other information displayed above the palette (such as peak height or peak area measured with the palette tools), text displayed in the Edit Menu and Experiment Setup dialog boxes, and the text used to display the Experiment drop-down list box, the System Status indicator and the Collect Status indicator. See “Palette” in the “About the Display” chapter and “Customizing the OMNIC menus” in this chapter for more information.
Spectrum Title	The title that appears in the title box of a spectral window when a displayed spectrum is selected. See “Title box” in the “About the Display” chapter.

Type	Description
Hidden Title	The title of a hidden spectrum that appears in the list of titles in a spectral window. See “Overlaying spectra” and “Stacking spectra” in the “About the Display” chapter for more information.
Gauge	Numbers that appear next to scrollable gauges, such as the subtraction factor scroll bar in the Subtract window.
Log Text	Text contained in a log. We recommend using a fixed-width font so that values contained in tables in the log will line up properly.

## Print options

The Print options appear when you click the Print tab.

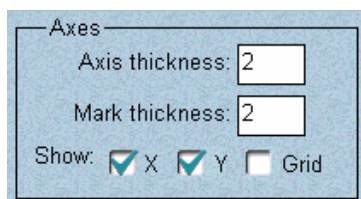


They affect how spectra and other images in spectral windows or in reports are printed on paper. The table below shows what you can specify.

To specify or do this...	Use this feature...
The thickness of printed axes.	Axis Thickness
The thickness of printed axis tick marks.	Mark Thickness

To specify or do this...	Use this feature...
Print the X-axis.	Show X
Print the Y-axis.	Show Y
Print a grid with spectra.	Show Grid
Print an information box with spectra.	Show Info Box
Print a box around spectra.	Show Outer Box
The margins for printing.	Margins
The line thickness of printed spectra.	Line Thickness
Print colors as patterns.	Show Colors As Patterns
The orientation of printed pages.	Orientation
The fonts for printing text.	Fonts

### Specifying how to print axes



The options in the Axes box affect how axes are printed. Specify the thickness of the lines used to print the axes by typing the desired value in the Axis Thickness text box. The thickness is measured in units that correspond to pixels on the screen. The allowed values are 1 through 6. For example, if the axes on the screen are two pixels thick (as set in the View options), you can print the axes with the same thickness by setting this option to 2.

Specify the thickness of the tick marks printed along the axes by typing the desired value in the Mark Thickness text box. The thickness is measured in units that correspond to pixels on the screen. The allowed values are 1 through 6.

If you want the X-axis (including its axis label and numbers) printed with spectra, turn on Show X. Similarly, turn on Show Y if you want the Y-axis printed.

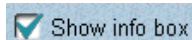
If you want a grid printed when you print spectra, turn on Show Grid. The grid is composed of vertical and horizontal lines that represent values on the X-axis and Y-axis. The major grid lines are aligned with tick marks, and the minor lines are evenly spaced between the major lines. The lines make it easier to find X and Y values of points in the spectra.

If Show Grid is on, a grid will be included if you print a spectrum displayed in a spectral window, or a log or report into which you have pasted a spectrum from any spectral window.

**Note** It is not necessary for a grid to be displayed to print spectra with a grid. ▲

If you are using paper that has a preprinted grid, turn off Show Grid. See “Specifying margins for printing” for details on printing on this type of paper.

### Printing an information box with spectra



Turn on Show Info Box if you want spectra in a spectral window printed with information about the selected spectrum in a box below the spectra. (If you want an information box printed for each spectrum, display each spectrum in a separate spectral window and then print each window.)

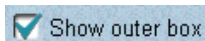
Six kinds of information will be included: the four items listed below plus the text in the Custom Info 1 and Custom Info 2 boxes in the Collection And Processing Information window. See “Collection and processing information” in the “About the Display” chapter for details.

- spectrum title
- date of collection
- resolution
- number of scans

**Note** If the spectrum title is long or you are using a large font size for printing sampling information, undesirable results may occur when you print an information box, especially if you print using portrait orientation. For best results, set Orientation to Landscape when Show Info Box is turned on. ▲

**Note** Show Info Box does not affect the printing of reports. ▲

### Printing a box around spectra



If you want a box drawn around printed spectra or other images, turn on Show Outer Box. If you are using paper that has a preprinted grid, it is usually best to turn off Show Outer Box before you print. See “Specifying margins for printing” for more information on printing or plotting on this type of paper.

## Specifying margins for printing

Margins (Inches)

Top:  Left:

Bottom:  Right:

The margins used for printing spectra or images on paper are shown in the Top, Bottom, Left and Right text boxes in the Margins (Inches) box. The margin values are in inches (some international versions of OMNIC use millimeters instead; this is set by Windows Control Panel).

If you are using paper with a preprinted grid, set the margins to correspond with the margins on the paper or to values that position the image at the desired location. You may need to experiment to determine the correct margin values for your paper.

Before you create a new report template with Template in the Report menu, use the options in the Margins box to set the margins for reports to be printed with the template. Once you create the template, you cannot change its margins.

## Specifying how to print spectra and other images

Spectra

Line thickness:  Orientation:

Show colors as patterns

Specify the thickness of the lines used to print spectra by typing the desired value in the Line Thickness text box in the Spectra box. The thickness is measured in units that are the equivalent of displayed pixels. If you have turned on Show colors as patterns (explained later in this section), the Line thickness option is not available.

Specify the thickness of the lines used to print spectra by typing a value in the Line Thickness text box. The thickness is measured in units that are the equivalent of displayed pixels. The allowed values are 1 through 10. If you have turned on Show Colors As Patterns (explained below), Line Thickness is not available.

If you want spectra that are displayed in different colors to be printed using different patterns to represent the colors, turn on Show Colors As Patterns. This feature is useful for overlaid spectra that would be hard to differentiate if printed on a black-and-white printer or if photocopied later. If you turn this option on, Line Thickness becomes unavailable and all the spectra are printed with line patterns (dashed lines, for example) having the same thickness.

Select the desired page orientation for printing from the Orientation drop-down list box: Landscape for a horizontal page or Portrait for a vertical page.

**Note** Changing the setting of the Orientation option does not reset the Orientation parameter in the Print Setup dialog box; however, the setting of Orientation in the Print options will be used when you print. Also, the page orientation setting in Windows Control Panel or in the printer setup dialog box for other applications is not affected by the setting you make here. See “Setting up the printer” in the “File” chapter for more information on the Orientation parameter. ▲

Before you create a new report template with Template in the Report menu, use the Orientation option to specify a portrait or landscape orientation for the reports. Once you create the template, you cannot change its orientation.

### Specifying fonts for printed text

The Fonts list box lets you specify which fonts, styles and sizes to use when printing various types of text. Each type is listed in the Type column of the list box and is described in the following table. The Style column indicates the font style used for each text type. The Size column shows the current font size in points. The Name column shows the current font name. The text types listed correspond to the types of the same name that you specify for displaying using the View options.

**Note** The font used to print text contained in the log window is the same font that is used to display the text. See “Specifying fonts for displayed text” for details. ▲

Text Type	Description
Annotation	Peak labels created using the palette tools or Find Peaks in the Analyze menu. Labels can include words and numbers.
Axis Labels	Axis labels showing the units of the X-axis.
Axis Numbers	Numbers that appear along the X-axis and Y-axis.
Sampling Info	Information about a spectrum contained in a pane and text contained in the printed information box (including the spectrum title, date of collection, resolution and number of scans). See “Printing an information box with spectra.”



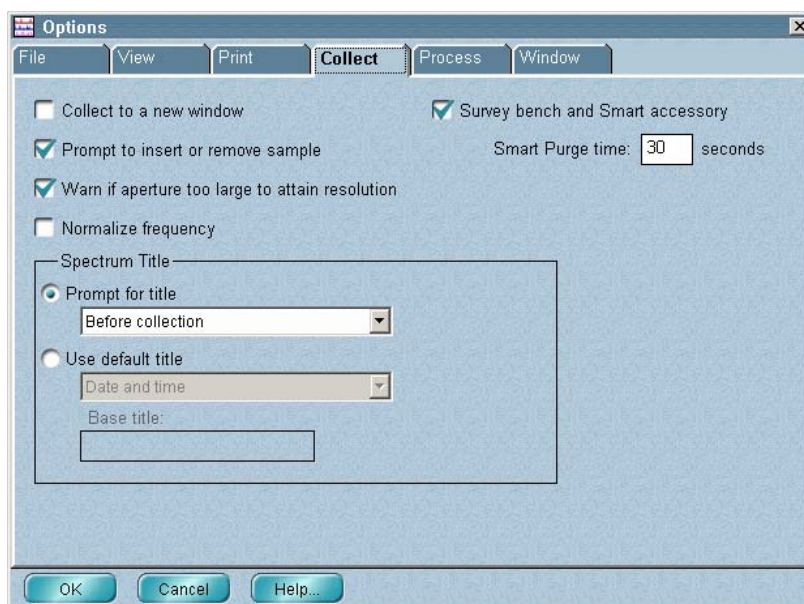
Text Type	Description
Spectrum Info	Information contained in the Custom Info 1 and Custom Info 2 boxes in the Collection And Processing Information window. (You can display this information by double-clicking a spectrum title in the title box.)



Using the Font button, you can change the font style, size and name for printing these text types in the same way as you specify fonts for displaying text on the screen. See “View options” for complete instructions.

### Collect options

The Collect options appear when you click the Collect tab.



They affect how spectra are collected. The table below shows what you can specify with each option.

To specify or do this...	Use this feature...
Place collected spectra into new spectral windows.	Collect To A New Window
Display prompts to insert and remove samples.	Prompt To Insert Or Remove Sample

To specify or do this...	Use this feature...
Display a warning if the aperture is too large for the selected resolution.	Warn If Aperture Too Large
Normalize the frequency automatically.	Normalize Frequency
How to title collected spectra.	Spectrum Title
Whether to monitor the operation of the spectrometer and check for the presence of a Smart Accessory.	Survey Bench And Smart Accessory
The duration of the increased purge flow rate for the Smart Purge option.	Smart Purge Time

### Placing collected spectra into new spectral windows

Collect to a new window

If you want collected spectra to be placed into a new spectral window automatically after each data collection, turn on Collect To A New Window. The new window will be given a default title. If you turn this option off, you will be asked whether to place the collected spectrum into a spectral window. See “Collecting a sample spectrum” and “Collecting a background spectrum” in the “Collect” chapter for details.

### Displaying prompts to insert and remove the sample

Prompt to insert or remove sample

Prompt To Insert Or Remove Sample lets you specify whether the software will prompt you to install or remove your sample at the appropriate time during data collection. The actual prompts that appear depend on the current setting of Background Handling in the Experiment Setup dialog box.

For example, if you are collecting a background spectrum before every sample spectrum and Prompt To Insert Or Remove Sample has been turned on, you will be prompted to prepare the system for background collection at the start of data collection. If you are collecting a background after every sample, you will be prompted to install your sample at the start of data collection. The same prompt will appear if you have set the software to collect a background after a specified time or if you are using a stored background. See “Background Handling” in the “Collect” chapter for more information on background handling.

If you don't want to be prompted, turn off Prompt To Insert Or Remove Sample. In this case, make sure the system is ready for background collection (if you are collecting a background first) or the sample is installed (if you are using any of the other Background Handling settings) before choosing Collect Sample from the Collect menu.

**Note** If you have turned off Prompt To Insert Or Remove Sample and are collecting a background before every sample, you will be prompted to install the sample after background collection. Similarly, if you are collecting a background after every sample, you will be prompted to clear the beam path after sample collection. ▲

### Displaying a warning if the aperture is too large

Warn if aperture too large to attain resolution

Warn If Aperture Too Large To Attain Resolution lets you specify whether the software will warn you if the aperture size is too large to achieve the specified resolution. (Increasing the aperture size reduces the resolution.) If the warning appears during data collection, use a smaller aperture or a lower resolution (higher setting of the Resolution parameter).

### Normalizing the frequency automatically

Normalize frequency

Normalize Frequency lets you specify whether the laser frequency of spectra you collect is automatically normalized. Normalizing the frequency changes the locations of the spectral data points to standard positions; that is, the positions they would be at if they had been collected using a spectrometer with a reference laser frequency of 15,798.0 wavenumbers. This results in better correspondence of data collected using spectrometers with slightly different laser frequencies.

Normalize the spectra of your standards and unknown samples if you are developing or using a quant method on more than one spectrometer. You should also normalize noncalibrated spectra; that is, JCAMP-DX spectra, spectra from CSV (comma-separated values) text files, and spectra collected using dispersive instruments.

The frequency is normalized only if it is not equal to the reference frequency and the difference between the two is less than 20 wavenumbers.

**Notice** Normalizing the frequency guarantees that data points occur at the same frequency positions. This lets you move data between spectrometers without the problems associated with inconsistent data point positioning. However, if you plan to analyze sample spectra using previously calibrated quant methods developed with a version of OMNIC earlier than 3.0, *do not normalize the frequency of the sample spectra*. If you normalize your sample spectra and attempt to use a calibrated method whose standards were not normalized, the data will not match and the analysis will fail. ▲

**Note** You can use Normalize Frequency in the File options to specify whether to normalize the frequency automatically when you open a spectrum. See “File options” for details. Use Normalize Frequency in the Process menu to normalize the laser frequency of a spectrum already displayed in a spectral window. See “Normalizing the frequency of a spectrum” in the “Process” chapter for details. ▲

When you normalize the frequency of a spectrum, a record of the operation is made in the “DATA PROCESSING HISTORY” section of the Collection And Processing Information window.

### Specifying how to title collected spectra

Use the options in the Spectrum Title box to specify whether the software will prompt you to enter a title for your sample spectrum or will use a default title. If you collect a series data set using OMNIC Series, these options affect how the data set is titled.

If you want to be prompted, select Prompt For Title and then select the desired option from the Prompt For Title drop-down list box. If you select Before Collection, the prompt will appear before the spectral data are collected. If you select After Collection, the prompt will appear after the data are collected.

To use a default spectrum (or series data set) title, select Use Default Title and then select the desired option from the Use Default Title drop-down list box.

The options described in the following table are available.

Option	Description
Date And Time	Titles will be the date and time of collection.
Auto Save Filename	The titles will be the same as their filenames if you are saving spectra automatically (Save Automatically is turned on in the Experiment Setup dialog box).
Auto Save Title	Titles will consist of a base title followed by a four-digit number. Type a base title in the Base Title text box. The number will increase by one with each sample spectrum (or series data set) you collect.
Auto Save Filename, Date And Time	The titles will consist of the base name (without an extension) specified in the Experiment Setup dialog box plus a four-digit number and the date and time of collection. The number will increase by one with each sample spectrum (or series data set) you collect. See “File handling” in the “Collect” chapter for more information.
Auto Save Title, Date And Time	Titles will consist of a base title followed by a four-digit number and the date and time of collection. Type the desired base title in the Base Title text box. The number will increase by one with each sample spectrum (or series data set) you collect.

### Surveying the spectrometer and Smart Accessory

Survey bench and Smart accessory

Select Survey Bench And Smart Accessory if you want the software to monitor the operation of the spectrometer and periodically check for the presence of a Smart Accessory. When this option is selected, the System Status indicator changes its appearance if a spectrometer problem is detected. See “Monitoring the spectrometer status” in the “About the Display” chapter for more information.

**Note** Turning off Instrument Status in the System Status Overview dialog box turns off Survey Bench And Smart Accessory. (Turning Instrument Status on does not turn on Survey Bench And Smart Accessory.) ▲

If you install a Smart Accessory when this option is selected, a message provides information about the accessory and lets you check its performance. Follow the instructions that appear on the screen.

### Setting Smart Purge

Smart Purge time:  seconds

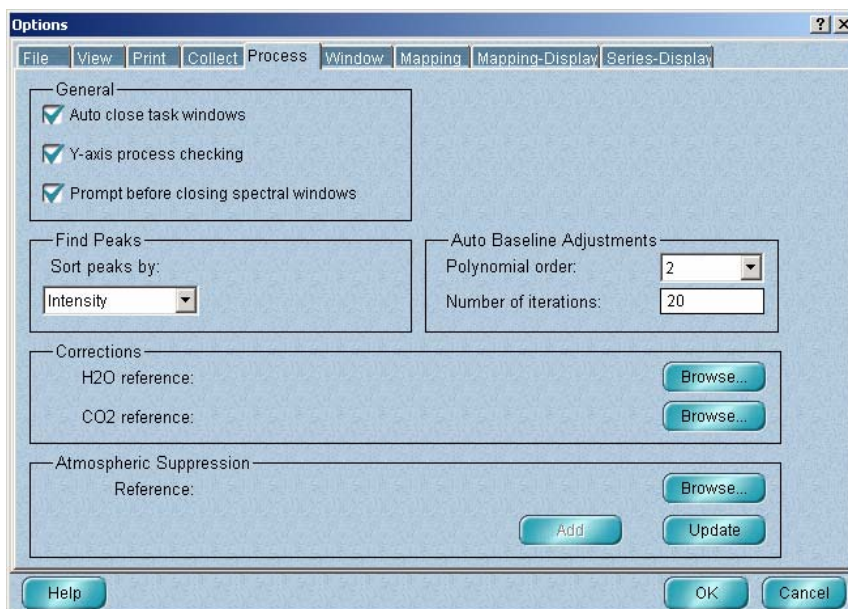
The Smart Purge™ option available on some spectrometer models increases the purge gas flow rate when you install or remove samples. This helps keep unwanted gases such as water vapor and carbon dioxide out of the spectrometer.

If you have the option, Smart Purge Time becomes available. To specify how long to purge the sample compartment at an increased rate, type the desired number of seconds, up to 250, in the text box. The period of increased purge flow begins when you open the sample compartment cover or sliding door. To disable Smart Purge, set Smart Purge Time to 0.

**Note** If you have an auxiliary experiment module (AEM) with Smart Purge, the duration of its increased purge flow is set at the factory and cannot be changed. ▲

### Process options

The Process options appear when you click the Process tab.



They affect several operations from the Process and Analyze menus. The table below shows what you can specify with each option.

To specify or do this...	Use this feature...
Close task windows automatically.	Auto Close Task Windows
Limit spectral data processing.	Y-Axis Process Checking
Whether to be prompted to save spectra before closing spectral windows.	Prompt Before Closing Spectral Windows
How to list peaks found by Find Peaks.	Sort Peaks By
Specify water and carbon dioxide reference spectra.	Corrections
Improve the results of the Automatic Atmospheric Suppression option (on the Collect tab of the Experiment Setup dialog box) by including your own reference spectrum in the mathematical model used by the option.	Atmospheric Suppression

### Closing task windows automatically

Auto close task windows

When you use some OMNIC commands, a task window is displayed to let you see the progress of an operation or to let you interact with the software. If you want task windows closed automatically after you place the task results into a spectral window, turn on Auto Close Task Windows. If the option is off, you will be asked whether to close the task window after you place the results in a spectral window. Leaving the window open lets you make further changes to the data. See “Task windows” in the “About the Display” chapter for more information on task windows.

### Limiting spectral data processing

Y-axis process checking

If Y-Axis Process Checking is turned on, the software checks the data formats being used and other conditions when you use Process menu commands (which affect the Y values of data points) and allows only normally performed actions to be carried out. If an operation is not considered normal because of the current conditions—for example, if you are attempting to subtract a spectrum from another spectrum with different Y-axis units—the software prevents the operation from being performed.

If this option is off, operations are performed regardless of the current data formats and conditions. (A message informs you of the irregularity.) This lets you perform operations in special situations in which the operations would normally not be allowed.

### Saving spectra before closing spectral windows

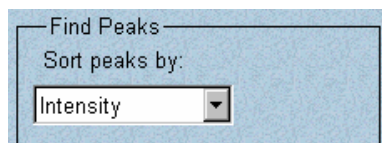
Prompt before closing spectral windows

Turn on Prompt Before Closing Spectral Windows if you want to be asked whether to save newly collected spectra and changes to spectral data contained in a spectral window when the window is closed. If this option is turned off, all unsaved data and changes to data in a spectral window will be lost when the window is closed.

### Note

If you have added annotation to a previously saved spectrum using the palette tools or Find Peaks in the Analyze menu but have not changed the spectral data, you will not be prompted when the spectral window is closed. Use Save in the File menu to save the annotation before closing the window. ▲

### Specifying how to list peaks found by Find Peaks

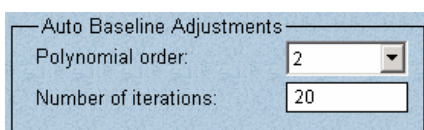


When you use the Print button or Clipboard button in the Find Peaks window to print or copy the results of a peak finding operation, a table listing the found peaks is printed or copied. To specify the order in which the peaks are listed, select an option from the Sort Peaks By drop-down list box.

- If you select Position, the peaks are listed in order of increasing wavenumber (X) value.
- If you select Intensity, the peaks are listed in order of decreasing intensity (Y) value.

See “Finding peaks” in the “Analyze” chapter for complete information on using Find Peaks.

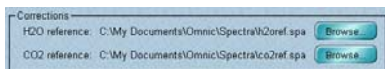
### Specifying the order and iterations for automatic baseline correction



Use Polynomial Order and Number Of Iterations to specify the order of the equation and number of iterations, respectively, to use for correcting baselines automatically with Automatic Baseline Correct in the Process menu. See “Correcting baselines automatically” in the “Process” chapter for more information.



## Specifying water and carbon dioxide reference spectra



The features in the Corrections box let you specify reference spectra to use for correcting sample spectra for the effects of water and carbon dioxide (see “Using Other Corrections” in the “Process” chapter for more information). To specify a water reference spectrum, click the Browse button to the right of H2O Reference. An Open dialog box lets you locate and select a file (by clicking its filename). When you choose OK, the pathname of the selected file appears below H2O Reference. Similarly, you can use the Browse button to the right of CO2 Reference to specify a carbon dioxide reference spectrum.

### Note for DS systems

If Prevent Changing Directories When Opening Files is selected in the system policies, you cannot change directories or drives to locate a file to select. ▲

### Notice

When you correct a spectrum later, the data spacing of the reference spectra will be adjusted to match the spectrum you are correcting. If possible, use the same resolution to collect the reference spectra as you will use for collecting the spectra you plan to correct. As an alternative, you can use the highest possible resolution to collect these spectra and save the interferograms with the spectra. The spectral ranges and processing parameter settings for the sample and reference spectra will match when the spectra are transformed from the interferograms. However, if you collect data at a high resolution, it will take more time to transform the data and correct the sample spectrum if the interferograms are used. ▲

*To collect a water reference spectrum:*

1. **Purge the spectrometer to remove water vapor and carbon dioxide.**
2. **Collect a background spectrum using Collect Background in the Collect menu.**

### Note

Collect at least 64 scans for both the background and sample reference spectra in this procedure to achieve a high signal-to-noise ratio. Collecting fewer scans can result in introduced noise in your corrected sample spectra. ▲

3. **Place an open container of water in the sample compartment and close the sample compartment cover.**

**4. Purge the spectrometer to remove any carbon dioxide.**

Water vapor will still be present since water continuously evaporates from the container.

**5. Collect a sample spectrum with no sample in place using Collect Sample in the Collect menu.**

Since the sample spectrum contains only water peaks, it can be used as a water reference.

*To collect a carbon dioxide reference spectrum:*

**1. Purge the spectrometer to remove water vapor and carbon dioxide.****2. Collect a background using Collect Background in the Collect menu.**

**Note** Collect at least 64 scans for both the background and sample reference spectra in this procedure to achieve a high signal-to-noise ratio. Collecting fewer scans can result in introduced noise in your corrected sample spectra. ▲

**3. Open the sliding door in the sample compartment cover about one centimeter, and gently blow carbon dioxide into the sample compartment using a cylinder of carbon dioxide and the appropriate fittings.****4. Quickly close the sliding door.****5. Collect a sample spectrum with no sample in place using Collect Sample in the Collect menu.**

Since the sample spectrum contains only carbon dioxide peaks, it can be used as a carbon dioxide reference.

This approach to correcting spectra is usually the easiest.

*To collect a water and carbon dioxide reference spectrum:*

1. **Purge the spectrometer to remove water vapor and carbon dioxide.**
2. **Collect a background using Collect Background in the Collect menu.**

**Note** Collect at least 64 scans for both the background and sample reference spectra in this procedure to achieve a high signal-to-noise ratio. Collecting fewer scans can result in introduced noise in your corrected sample spectra. ▲

3. **Open the sample compartment cover.**
4. **Collect a sample spectrum with no sample in place using Collect Sample in the Collect menu.**

Since the sample spectrum contains water and carbon dioxide peaks, it can be used only to correct spectra for both water and carbon dioxide. To use this spectrum as a reference, specify it as both the water and carbon dioxide references in the Process options, and set Correction to H2O And CO2 in the Experiment Setup dialog box (see “Selecting a correction type” in the “Collect” chapter).

### Specifying an additional reference for atmospheric suppression



If you find that the Automatic Atmospheric Suppression option on the Collect tab of the Experiment Setup dialog box does not adequately suppress the effects of water vapor and carbon dioxide absorptions in the sample spectra you collect, you can use the features in the Atmospheric Suppression box to improve your results. The Automatic Atmospheric Suppression option uses a quantitative model to suppress water and carbon dioxide effects. You can improve this model by collecting your own reference spectrum and including it when the model is generated.

When you collect the spectrum, use the following parameter settings in the Experiment Setup dialog box:

- Set Resolution to 0.5 on the Collect tab. If the highest resolution (smallest numerical setting) available for your spectrometer is 1 wavenumber, use that setting instead.

- Set Final Format on the Collect tab to Absorbance or %Transmittance.
- Turn on Save Interferograms on the Collect tab.

Collect your reference spectrum without a sample installed, under the same environmental conditions as will exist when you later collect your sample spectra. Save the spectrum and then use the Browse button in the Atmospheric Suppression box on the Process tab to locate and select the spectrum.

**Note for DS systems**

If Prevent Changing Directories When Opening Files is selected in the system policies, you cannot change directories or drives to locate a spectrum to select. ▲



After you select the spectrum and choose Open, its pathname appears in the Atmospheric Suppression box. To include this spectrum when the model is calculated, choose Add. You can repeat this process (using the Browse button and then the Add button) to include more than one additional reference spectrum in the model. The next time you collect a spectrum with Automatic Atmospheric Suppression turned on, the model will be used.



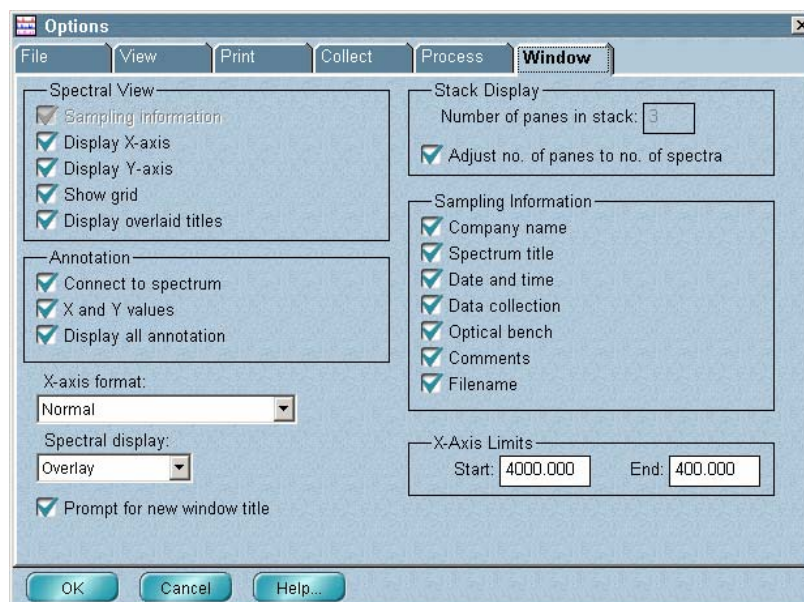
If you want all of the currently stored models recalculated using the reference spectrum, choose Update. The calculations can take a long time if you have a number of models.

**Note**

The first time you use the new model, data collection will be delayed while the method is recalibrated. ▲

## Window options

The Window options appear when you click the Windows tab.



They affect the way spectra and other information will be displayed in new spectral windows. A new spectral window is created when you use New Window in the Window menu or use the window selection box to add a result spectrum from a task window to a new window. See “Creating a new spectral window” in the “Window” chapter or “Task windows” in the “About the Display” chapter for more information.

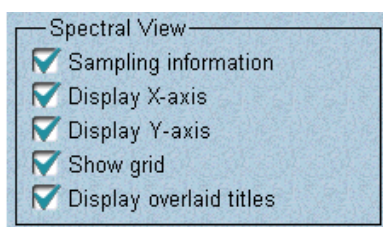
**Note** The Window options settings serve as the defaults for new spectral windows. You can change the way information is displayed in a window by using Display Setup in the View menu or the View options. See “Setting the display parameters” in the “View” chapter and “View options” in this chapter for details. ▲

The table below shows what you can specify with each option.

To specify or do this...	Use this feature...
Display sampling information.	Sampling Information
Display the X-axis.	Display X-Axis
Display the Y-axis.	Display Y-Axis
Display a grid with spectra.	Show Grid

To specify or do this...	Use this feature...
Display overlaid spectrum titles.	Display Overlaid Titles
Connect annotation to spectra with a line.	Connect To Spectrum
Include both X and Y values in labels created with the annotation tool.	X And Y Values
Display annotation for all spectra.	Display All Annotation
The X-axis format for new spectral windows.	X-Axis Format
Whether to overlay or stack spectra.	Spectral Display
Whether to be prompted for a window title when a new spectral window is created.	Prompt For New Window Title
The number of panes to use when displaying stacked spectra.	Number Of Panes In Stack
Adjust the number of panes in a stack to match the number of spectra.	Adjust Number Of Panes To Number Of Spectra
The sampling information to display.	Sampling Information
The X-axis display limits for new spectral windows.	X-Axis Limits

## Spectral View

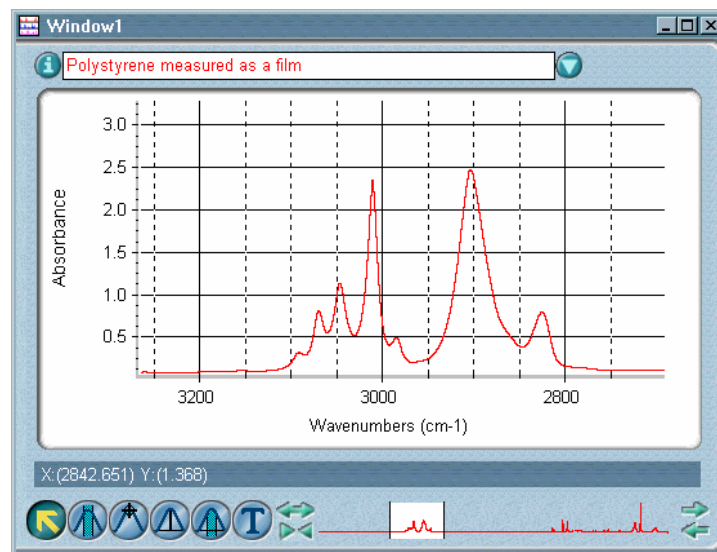


If you want sampling information displayed with spectra in new spectral windows, turn on Sampling Information. The kinds of information selected in the Sampling Information box will be displayed. See “Specifying the sampling information to display” for details on selecting the kinds of information to display.

If you want the X-axis displayed in new spectral windows, turn on Display X-Axis. If you want the Y-axis displayed in new spectral windows, turn on Display Y-Axis.

If you want a grid displayed when you display spectra in a new spectral window, turn on Show Grid. The grid is composed of vertical and horizontal lines representing values on the X-axis and Y-axis. The major grid lines are aligned with the tick marks labeled with axis values, and the minor lines are evenly spaced between the major lines. The lines make it easier to find X and Y values of data points. The thickness of the grid lines is always one pixel.

Here is an example:

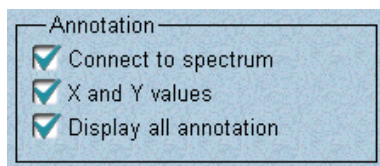


To remove the grid from a spectral window, turn off Show Grid in the Display Setup dialog box. See “Displaying a grid” in the “View” chapter.

**Note** If you want a grid to be printed with spectra or included when you paste a spectrum into a log, turn on Show Grid in the Print options. See “Specifying how to print axes” in this chapter. ▲

If you want the titles of all the overlaid spectra in a new spectral window to be displayed at all times (except for hidden spectra, turn on Display Overlaid Titles.

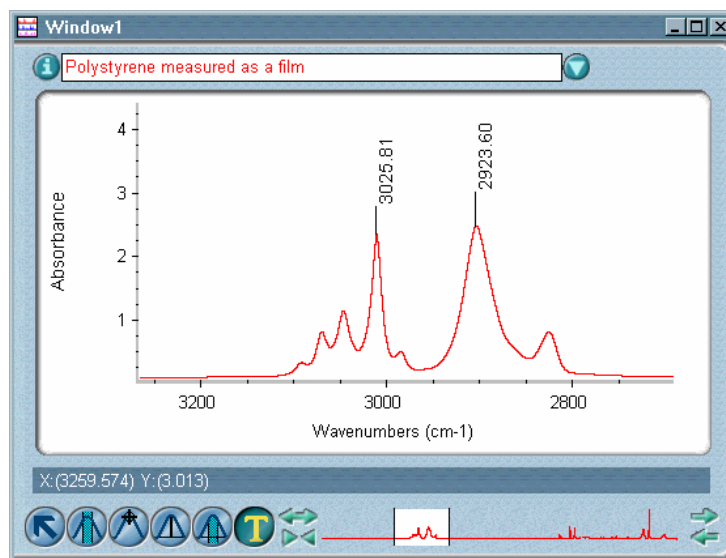
### Specifying how to display annotations in new spectral windows



Use the options in the Annotation box to specify how to display labels and other annotation in new spectral windows.

Turn on Connect To Spectrum if you want new annotations you create with the palette tools to be connected to the spectra with a line. (A label created using Find Peaks in the Analyze menu will always be connected to the spectrum with a line if you move the label away from the spectrum.)

Here is an example:

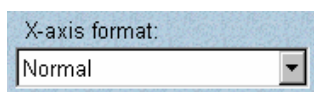


Turn on X And Y Values if you want to display both the X and Y values of the point you are annotating with the annotation tool instead of just the X value. (You can still edit the annotation after you create it.)

Turn on Display All Annotation if you want to display the annotations and labels for all the displayed spectra in the spectral window instead of just for the selected spectrum.

**Note** You can display annotations vertically or horizontally and specify a font for the text by using the View options. ▲

### Specifying an X-axis format for new spectral windows



Select the X-axis format you want to use for new spectral windows from the X-Axis Format drop-down list box. See “Selecting an X-axis format” in the “View” chapter for a description of the available formats.

### Overlaying or stacking spectra in new spectral windows



If you want spectra in new spectral windows to be overlaid, select Overlay from the Spectral Display drop-down list box. If you want the spectra to be stacked, select Stack. (You will still be able to change between overlaying and stacking spectra using Stack Spectra and Overlay Spectra in the View menu.)



## Displaying a prompt for titling new spectral windows

Prompt for new window title

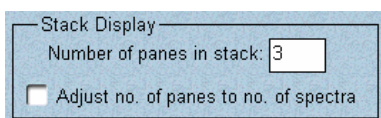
Prompt For New Window Title lets you specify whether you will be prompted to enter a window title in the following situations:

- You use New Window in the Window menu to create a new spectral window. See “Creating a new spectral window” in the “Window chapter” for more information.
- You add the result spectrum from a task window to a new spectral window.
- You add a library spectrum to a new spectral window using Library Manager. See “Placing a library spectrum into a spectral window” in the “Analyze” chapter for details.

When the prompt appears, type the desired title in the text box and then choose OK. To use the default title shown in the text box, just choose OK.

If you want to be prompted, turn on Prompt For New Window Title. To use the default title for new spectral windows, turn this option off. The default title is “Window” followed by a number; for example, “Window2.” The number increases by one with each new spectral window you create.

## Specifying how to stack spectra in new spectral windows



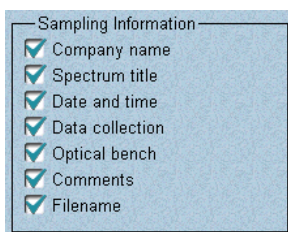
The options in the Stack Display box affect stacked spectra. Use Number Of Panes In Stack to specify the number of panes to display in new spectral windows when you stack spectra using Stack Spectra in the View menu. Typically two panes are stacked for visually comparing spectra.

If there are more spectra in the window than panes, a scroll bar at the right lets you scroll spectra into view. If there are more panes than spectra, some panes will be empty. This option is not available if Adjust Number Of Panes To Number Of Spectra is turned on (explained below).

Turn on Adjust Number Of Panes To Number Of Spectra if you want the number of panes in a stack adjusted automatically to match the number of displayed (not hidden) spectra instead of using the number specified by Number Of Panes In Stack. This lets you see every displayed spectrum in the window without using the stack scroll bar; keep in mind, however, that the panes become smaller as you add spectra.

See “Stacking or overlaying spectra” in the “View” chapter and “Stacking spectra” in the “About the Display” chapter for more information.

## Specifying the sampling information to display in new spectral windows



If you selected Sampling Information in the Spectral View box, the selected kinds of information in the Sampling Information box (described below) will be displayed when you display spectra in a new spectral window. (Both the Sampling Information option and the desired items in the Sampling Information box must be turned on for sampling information to be displayed.) All the listed kinds of information are originally saved when you save a spectrum following data collection. To change which information will be displayed, turn the appropriate check boxes on or off.

Item	Description
Company Name	The company name entered when the software is installed.
Spectrum Title	The title of the displayed spectrum.
Date And Time	The date and time the spectrum was collected.
Data Collection	
Sample Scans	The number of sample scans collected.
Background Scan	The number of background scans collected.
Resolution	The resolution used for sample and background data collection.
Gain	The gain used to amplify the detector signal.
Optical Velocity	The optical velocity.
Aperture	The relative size of the aperture expressed as a percent of maximum area.
Optical Bench	
Detector	The type of detector used.
Beamsplitter	The type of beamsplitter used.
Source	The type of source used.
Accessories	The accessories used to collect the spectrum.
Comments	Any comments about the spectrum that you have recorded in the Collection And Processing Information window.
Filename	The filename of the spectrum.
System Status Results	

See “Spectral View” for a description of the Sampling Information option.

## Specifying X-axis display limits for new spectral windows



You can specify the X-axis limits for displaying spectra in new spectral windows by typing the desired values in the Start and End text boxes in the X-Axis Limits box. The most commonly used starting and ending limits for wavenumbers are 4000 and 400, respectively. See “Specifying an X-axis format” for information on selecting an X-axis format.

### ■ *How to* ➔

Set the options

#### 1. Choose Options from the Edit menu.

The Options dialog box appears.

#### 2. Display the set of options you want to change by clicking the appropriate tab at the top of the dialog box.

#### 3. Set the options as desired.

#### 4. Repeat steps 2 and 3 for the other options you want to change.

#### 5. When you are finished setting the options, choose OK.

## Customizing a menu

The Edit Menu command in the Edit menu allows you and other users to customize the contents of the OMNIC menus for the way each person prefers to use the software. You can enable, disable, hide, add, delete and modify items in the menus.

### Note for DS systems

Access to standard menu items is controlled by the Security Administration software, regardless of any changes you make with Edit Menu. You can still add items, such as macros, to a menu. ▲

### Note

You can disable, but not hide, commands in cascading menus. These menus appear when you point to items in the Help menu that have an arrow symbol to the right of the item name. ▲

After you customize the menus, you can save your menu configuration in a configuration file that can be opened later. This lets you quickly reset OMNIC to your preferences after others have used the software. You can assign a password to protect the file so that only you can make changes to the configuration. See “Saving a configuration” and “Opening a configuration” in the “File” chapter for more information.

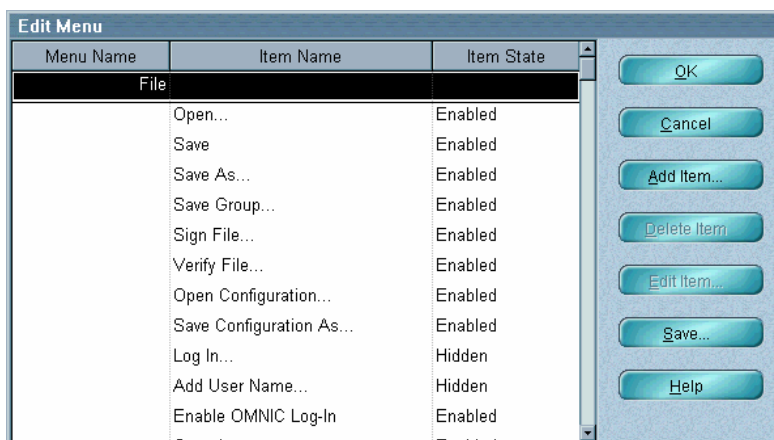
**Note** You can hide all of the menus by turning on Hide All OMNIC Menus in the Edit Toolbar dialog box. See “Customizing a toolbar” for details. ▲

➤ **How to** ➡ Customize menus

**1. Choose Edit Menu from the Edit menu.**

The Edit Menu dialog box lists every item in each OMNIC menu and the current state of each item.

The scroll bar to the right of the columns lets you scroll through the menus and menu items.



The following table describes the three possible states of any item.

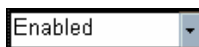
State	Description
Enabled	Displayed in the menu and available for use.
Disabled	Displayed in the menu but dimmed (not available for use).
Hidden	Not displayed in the menu and not available for use.

**Note** The font used for text in this dialog box is determined by the Readout text type in the View options. See “Specifying fonts for displayed text” in the “Edit” chapter. ▲

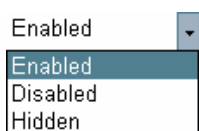
**Note** You can disable, but not hide, commands in cascading menus. ▲

## 2. Change the state of the menu items as desired.

To change the state of an item, first double-click the text (“Enabled,” “Disabled” or “Hidden”) indicating the current state in the Item State column. An arrow button appears to the right.



Click the arrow button. A drop-down list box appears.



Select the desired State.

### Note for DS systems

Access to standard menu items is controlled by the Security Administration software, regardless of any changes you make with Edit Menu. You can still add items, such as macros and external programs (see the next step), or change the state of added items. The user can run an added macro, program or DDE command only if allowed to do so by the Run Macros From Menu Or Toolbar policy, Run Programs Form Menu Or Toolbar policy, or Use DDE Commands From Menu Or Toolbar policy, respectively. ▲

## 3. To add an item to a menu, choose Add Item.

You can add an item to a menu for initiating a macro, an external application (such as a spreadsheet or word processing program) or an OMNIC DDE (dynamic data exchange) command. The Menu Item dialog box appears.

Select the desired item type in the Item Type box and enter the needed information in the text box at the bottom of the dialog box. The available types and needed information are described in the following table.

**Note for DS systems**

If Prevent Changing Directories When Opening Files is selected in the system policies, you cannot change directories or drives to locate a macro or program file to select (see the instructions below). ▲

Item Type	Description	Needed Information
Run Basic Macro	Runs a macro created using OMNIC Macros\Basic.	Enter the pathname of the macro, or use the Browse button to locate and select the needed macro.
Run External Program	Starts another application.	Enter the pathname of the external application, or use the Browse button to locate and select the needed program file.
Execute DDE Command	Executes a DDE command available in OMNIC Macros\Pro.	Text of the DDE command.

Select from the Menu drop-down list box the menu to which you want the item added.

Type in the Menu text box the name of the item exactly as you want it to appear in the menu.

When you are finished specifying the item, choose OK. The item then appears at the end of the list of items for the specified menu.

#### 4. Delete any items you want removed from the menus.

You can delete any item that you have added to a menu; you cannot delete a standard OMNIC menu item. To delete an item, select it and then choose Delete Item. (You can use the up and down arrow keys on the keyboard to select items.) The item is removed from the list.

**5. If desired, edit any of the items that have been added to the menus.**

You can edit any item that has been added with the Add Item button, either during this work session or in the past. You cannot edit a standard menu item.

The Menu Item dialog box appears. Make the desired changes using the instructions given in step 3. When you are finished, choose OK.

**6. If you disabled or hid the Save Configuration As command and want to save your changes, click the Save button.**

(You will not be able to save your changes after closing the Edit Menu dialog box in this case.) The Save Configuration dialog box appears. This is the same dialog box that appears when you choose Save Configuration As from the File menu. See “How to save a configuration” in the “File” chapter for instructions on using the dialog box; start with step 2 of that procedure.

**7. When you are finished customizing the menus, choose OK.**

To save your menu changes, use Save Configuration As in the File menu (if it is available).

## Customizing a toolbar

Edit Toolbar in the Edit menu lets you and other users create custom toolbars containing buttons for quickly initiating commands, macros or external programs. You can create a button for any command in any OMNIC menu.

### Note for DS systems

A command button in the toolbar is active only if the logged-on user has access rights to use the corresponding menu command. The user can still add items, such as macros, to the toolbar. ▲

You can remove the menu bar and Experiment drop-down list box from the OMNIC window by turning on the Hide All OMNIC Menus option. This lets you create a simplified configuration in which users must use toolbar buttons instead of menu commands to perform operations.

**Notice** If you turn on Hide All OMNIC Menus, do *not* turn on Set As Default Configuration when you save the configuration with the Save button. ▲

**Note** If you turn on Hide All OMNIC Menus, the Add To A New Window option will not be available in the window selection box in task windows. ▲

After you create a toolbar, you can save it as part of your own software configuration in a file that can be opened later. (The setting of Hide All OMNIC Menus is also saved in the configuration.) This lets you quickly reset OMNIC to your preferences after others have used the software. You can assign a password to protect the file so that only you can make changes to the configuration. See “Saving a configuration” and “Opening a configuration” in the “File” chapter for details on saving and opening a configuration file.

## — *How to* ➔ Customize a toolbar

### 1. Choose Edit Toolbar from the Edit menu.

The Edit Toolbar dialog box appears.





The Button Library box shows the standard buttons that you can add to the toolbar. To see the command name for a button, point to the button and wait a moment. To see the buttons that are currently out of view, use the scroll bar below the buttons. The first button in the row contains a vertical dividing line and is used to separate groups of buttons in the toolbar.

The Current Toolbar box shows the buttons that are assigned to the toolbar for the current software configuration. As with the button library above, you can point to these buttons to see their names. To see buttons that are out of view, use the scroll bar below the buttons.

**Note for DS systems**

A command button in the toolbar is active only if the logged-on user has access rights to use the corresponding menu command. The user can still add items, such as macros and external programs, to the toolbar. The user can run an added macro, program or DDE command only if allowed to do so by the Run Macros From Menu Or Toolbar policy, Run Programs Form Menu Or Toolbar policy, or Use DDE Commands From Menu Or Toolbar policy, respectively. ▲

2. **If you want to use the default toolbar, choose Load Default.**
3. **If you want to add a standard button or space to the toolbar, drag it from the button library to the desired location in the current toolbar.**
4. **If you want to remove an item from the current toolbar, drag it to the trash can.**



- 5. Specify the size of the toolbar buttons by selecting Small or Large in the Button Size box.**

Using small buttons allows more of them to be displayed in the OMNIC window, but the images on the buttons may be harder to discern. The size change takes effect when you choose OK to close the Edit Toolbar dialog box.

- 6. Specify where within the OMNIC window to display the toolbar by selecting an option in the Toolbar Location box.**

- 7. If you want to remove the menu bar and Experiment drop-down list box from the OMNIC window, turn on Hide All OMNIC Menus.**

- 8. Specify what you want to appear on the toolbar buttons by selecting Icon, Icon And Text, or Text Only in the Button Style box.**

If you select an option that displays text, the text on a button will match the corresponding command name in the menu. (If the full command name is too long to fit on the button, the name is abbreviated.) The text on a custom button will be the specified button name.

- 9. If desired, use the features in the User Item box to create and add a custom button to the toolbar for initiating a macro, an external application (such as a spreadsheet or word processing program) or an OMNIC DDE (dynamic data exchange) command.**

You can use button images that are bitmaps created using a graphics program (such as a bitmap editor or icon editor), clip art or icons provided with an external application. A number of icons that you can use are provided in the Icons directory within the OMNIC directory.

To add a custom button to the toolbar, choose Add Item. The Add Toolbar Item dialog box appears. Select the desired item type in the Item Type box and enter the needed information in the text box below the Item Type box.

The available types and needed information are described in the table below.

Item Type	Description	Needed Information
Run Basic Macro	Runs a macro created using OMNIC Macros\Basic.	Pathname of the macro.
Run External Program	Starts another application.	Pathname of the external application.
Execute DDE Command	Executes a DDE command available in OMNIC Macros\Pro.	Text of the DDE command.

If you select Run Basic Macro or Run External Program, the Browse button becomes available in the Item Type box. You can choose Browse to display a dialog box that lets you locate and select the needed macro or program file.

**Note for DS systems** If Prevent Changing Directories When Opening Files is selected in the system policies, you cannot change directories or drives to locate a macro or program file to select. ▲

Type the name of the button in the Item Name text box. When you later point to the button in the toolbar in the OMNIC window, this name will appear.

To specify the appearance of the button, click the Browse button in the Icon/Bitmap box. A dialog box lets you select a file that contains a bitmap or icon image. (A number of icons are provided with OMNIC and are located in the Icons directory within the OMNIC directory.) When you select a file, the image it contains appears as a button below the word "Button." Choose OK after you select the desired file. The new button appears in the Icon/Bitmap box.

**Note** You can create an image for a button by using a paint program or other program that lets you create and save images as bitmaps (with the file extension .BMP) or icons (with the file extension .ICO). The size of the image should be 32 by 32 pixels. ▲

Choose OK to close the Add Toolbar Item dialog box.

The new button appears in the User Item box. To add the button to the toolbar, drag it to the desired location in the current toolbar.

After you add a custom button, you can edit the button by double-clicking it. The Edit Toolbar Item dialog box appears, and you can then use the same techniques to edit the button as you did to create it. When you choose OK to close the dialog box, any changes you made to the appearance of the button are displayed in the current toolbar in the Edit Toolbar dialog box.

**10. If you turned on Hide All OMNIC Menus and want to save your toolbar in a configuration file, use the Save button.**

You will not be able to use Save Configuration As in the File menu to do this, since the menu will not be available.

The setting of Hide All OMNIC Menus will also be saved in the configuration. In the Save Configuration dialog box enter a filename for the configuration and then choose Save. Do *not* turn on Set As Default Configuration when you save the configuration.

**Note for DS systems**

You may be prompted to digitally sign a file during this step. Follow the instructions that appear on the screen. If you are not prompted but want to sign the file, turn on Use Digital Signature in the Save Configuration dialog box. ▲

**11. When you are finished customizing the toolbar, choose OK.**

The customized toolbar appears in the OMNIC window if you have used Toolbar in the View menu to turn on the display of the toolbar. See “Displaying and using a toolbar” in the “View” chapter for more information.

If the specified buttons do not all fit in one column or row in the OMNIC window, additional columns or rows are used.

To save your toolbar changes, use Save Configuration As in the File menu.

# Collect

The Collect menu includes commands for preparing the system for data collection and collecting spectra. The table below summarizes the main use of each command:

To do this...	Use this command...
Set the data collection parameters, perform diagnostic checks or align the spectrometer.	Experiment Setup
Set the data collection and spectrometer parameters to the values that were used to collect the selected spectrum.	Match Spectrum Settings
Display an image of the spectrometer's optical components, view the path of the infrared beam and select a detector.	Show Optical Layout
Collect a sample spectrum.	Collect Sample
Collect a background spectrum.	Collect Background
Display the current background spectrum.	Display Background
Display a copy of the current spectral quality reference spectrum.	Display Spectral Quality Reference
Designate a background spectrum as the spectral quality reference spectrum for the current Smart Accessory experiment.	Set New Spectral Quality Reference
Start the Bench Diagnostics software to check spectrometer performance.	Advanced Diagnostics

You can customize the way OMNIC collects data by setting options using the Options command in the Edit menu. See “Customizing OMNIC by setting options” in the “Edit” chapter for details.

## Selecting an experiment

Before you collect a spectrum, you can set up the software for your application in one step by selecting an experiment from the Experiment drop-down list box near the top of the OMNIC window. This automatically sets the features in the Experiment Setup dialog box for your application, eliminating the need to set them individually. If you want to check or change the settings of the features, use Experiment Setup in the Collect menu. See “Using Experiment Setup” for details.

**Note** This feature is available only if Hide All OMNIC Menus is turned off in the Edit Toolbar dialog box (available through the Edit menu). ▲

When you install a Smart Accessory, the appropriate experiment is automatically selected for you and appears in the Experiment drop-down list box. (If Hide All OMNIC Menus is turned on, you must use the Smart Accessory, if any, that is required for the current experiment. If you install a different Smart Accessory, a prompt asks you to replace it.)

The experiment you select also sets the parameters in the Library Setup dialog box (except for those on the Library Directories tab) and the parameters in the QCheck Setup dialog box. See “Setting up a spectral search or QC comparison” in the “Analyze” chapter for complete information about Library Setup. See “Setting up a QCheck comparison” in that chapter for information about QCheck Setup.

The experiments shown in the Experiment drop-down list box are those in the current experiment directory that have been opened by using Experiment Setup or by installing a Smart Accessory. If the current experiment directory is OMNIC\Param, the Default experiment provided with OMNIC is also shown. You can change the experiment directory when you save an experiment using the Save As button in the Experiment Setup dialog box, but we recommend that you keep all your experiments in the same directory, preferably OMNIC\Param.

We recommend saving an experiment for each of your commonly used applications. Several example are provided with OMNIC.

**Note** You can also select an experiment by using the Open button in the Experiment Setup dialog box. You can open a parameter file from an early version of OMNIC (3.0 or earlier) by first selecting the Parameter Files file type (\*.PRM) in the Open Experiment dialog box. ▲

## Using the provided example experiments

The example experiments provided with OMNIC contain parameter settings appropriate for use with various OMNIC tutorials and for collecting spectra using different applications. When you select an experiment file in the Open Experiment dialog box (displayed when you choose Open in the Experiment Setup dialog box), its title and description appear making it easier find an appropriate experiment.

When you install a Smart Accessory, the appropriate experiment is automatically selected for you (or a list of appropriate experiments is made available for your selection), and you can begin collecting spectra. You can also select an experiment by selecting its title from the Experiment drop-down list box (if available) near the top of the OMNIC window or by using the Open button in the Experiment Setup dialog box. See “Selecting an experiment” or “Using Experiment Setup” for more information.

**Note** The experiments shown in the Experiment drop-down list box are those in the current experiment directory that have been opened by using Experiment Setup or by installing a Smart Accessory. You can open any available experiment by using the Open button in the Experiment Setup dialog box. ▲

## Restoring the default settings

If you have changed the parameter settings in one of the provided experiments and want to restore the parameters to their default settings, follow these steps:

- 1. Use the Open button in the Experiment Setup dialog box to open the experiment whose parameter settings you want to restore.**

See “Using Experiment Setup” for more information.

- 2. If you want to keep a copy of the current version of the experiment, use the Save As button to save it using a new filename.**

Otherwise, the experiment will be overwritten in step 4.

- 3. Use the Open button to open the experiment in the Factory directory (located in the OMNIC\Param directory) whose filename is the same as the original filename of the experiment you saved in step 2.**

This experiment contains the default settings.

4. Use the **Save As** button to save the experiment in the desired directory; normally this is the OMNIC\Param directory.

Do not change the experiment filename.

### Note for DS systems

If Prevent Changing Directories When Saving Files is selected in the system policies, you cannot change directories or drives when saving an experiment. ▲

You can now use the restored experiment for running the appropriate tutorial or for collecting spectra using an appropriate application.

## System Performance Verification

System Performance Verification (SPV) provides the following set of features for monitoring the performance of your system and the quality of collected spectral data. (Some of these features may not be available for your system.)

**Instrument Status** monitors the operation of key spectrometer components.

**System Suitability** lets you test the suitability of your spectrometer for your application by using tests and acceptance limits that you specify.

**Performance Verification** lets you check the operation of your spectrometer to verify that it passes several ASTM E-1421 based performance tests. This feature is available only if ValPro Qualification is not installed.

**ValPro Qualification** is an optional package that includes extensive documentation and procedures that let you qualify and check the operation of your spectrometer using pharmacopeial-recommended performance tests. This option allows you to compare the current qualification results with those obtained in the past to see trends in system performance.

**Scheduled Maintenance** lets you set up scheduling of system maintenance and be informed when maintenance needs to be performed.

**Spectral Quality** lets you see the results of the last performed spectral quality checks.



To access all installed SPV features, including options for configuring and enabling monitoring for features, choose Configure System Status from the View menu. To view results of SPV monitoring without the setup features, click the System Status indicator near the top of the OMNIC window. (You can also choose System Status from the View menu.) The indicator's appearance changes to show the status of test results for the SPV features currently being used to monitor system operation. (The indicator is not affected by the status of spectral quality checks reported by Last Spectral Quality Result.)

**Note** You can control access to the SPV setup features. If you have OMNIC DS, use the Security Administration software for this (see “Controlling access to client application features” in the *Security Administration User's Guide*.) If you do not have OMNIC DS, use Edit Menu in the Edit menu in conjunction with OMNIC configuration files and user log-ins to limit access. ▲

When the System Status Overview dialog box appears, it lists the available SPV features and shows their current status:



If this icon appears to the left of an SPV feature, the status is good and no action is needed.



If this icon appears to the left of an SPV feature, a problem was detected but it is not serious. The problem may require a corrective action.



If this icon appears to the left of an SPV feature, a serious problem was detected and corrective action is needed.

If you used Configure System Status to display the dialog box, you can enable or disable monitoring of an SPV feature by clicking its name and setting Monitoring to On or Off. If other features appear, you can use them to run a test, set up the SPV feature, view test results, etc. Complete information about each SPV feature is provided in the next sections.

## Viewing the system status

Choose System Status from the View menu to display the System Status Overview dialog box. It gives you access to some of the System Performance Verification features, such as running tests. (You can also click the System Status indicator near the top of the OMNIC window.)

**Note** To access all of the features, including options for configuring and enabling monitoring for features, choose Configure System Status (if available) from the View menu. ▲

## Controlling access to System Performance Verification features

Configure System Status in the View menu provides access to the System Status Overview dialog box with all installed features present, including options for configuring and enabling monitoring for System Performance Verification features. If you do not have OMNIC DS, you can use Edit Menu in the Edit menu to control access to these setup features in the dialog box. This lets you limit particular users to running performance tests and using a reduced set of features.

### Note for DS systems

If you have OMNIC DS, access to the Configure System Status and System Status commands in the View menu is controlled by the Security Administration software rather than through the procedure below. See “Controlling access to client application features” in the *Security Administration User's Guide* for more information. ▲

To prevent particular users from using Configure System Status:

1. **With Configure System Status available in the View menu, save the current OMNIC configuration with a password and a unique file name.**
2. **Use Edit Menu in the Edit menu to disable or hide the Configure System Status command and the Edit Menu command.**
3. **Save the configuration with a password and a different file name.**

Only users who know the password will be able to open the configuration that gives access to Configure System Status. Other users will be limited to using a version of the System Status Overview dialog box that does not include the setup features.

## Monitoring spectrometer components with Instrument Status

The Instrument Status feature of System Performance Verification lets you monitor the operation of several spectrometer components. The components that can be monitored depend on your spectrometer model.

If you use Configure System Status in the View menu to display the System Status Overview dialog box, you can enable monitoring by clicking Instrument Status, setting Monitoring to On and choosing OK.

**Note** Setting Monitoring to Off turns off Survey Bench And Smart Accessory in the Collect options. (Setting Monitoring to On does not turn on Survey Bench And Smart Accessory.) ▲

When monitoring is enabled, the appearance of the System Status indicator reflects the results of system diagnostic tests:



If the spectrometer has passed all of its tests, the System Status indicator shows a green check mark.



If the System Status indicator shows a yellow icon containing an exclamation mark, a cooled detector has become warm or data cannot be collected because the printer port is being used to print information (on some systems).



If the System Status indicator shows red “X,” the spectrometer has failed a test and requires corrective action or the computer cannot communicate with the spectrometer.

For help with solving the problem, click the indicator, click Instrument Status in the System Status Overview dialog box and click the Explain Error button.

## **Scheduling System Suitability, Performance Verification and ValPro Qualification tests and system maintenance**

You can specify the interval after which System Suitability, Performance Verification or ValPro Qualification tests (if available for your system) or system maintenance must be performed by setting the expiration period or date for the current test results. Follow these steps:

1. **Choose Configure System Status from the View menu.**
2. **Click the item whose expiration you want to set (System Suitability, Performance Verification, ValPro Qualification or Scheduled Maintenance) in the System Status Overview dialog box (displayed by choosing Configure System Status from the View menu).**

**3. Click the Set Interval button.**

A dialog box appears.

**4. Set the expiration for the item's test results or for system maintenance.**

- To specify an expiration interval of one or more months, select the first option and then select the desired number of months and the day of the month the expiration occurs.
- To specify an expiration interval of one or more weeks, select the second option and then select the desired number of weeks and the day of the week the expiration occurs.
- To specify an expiration interval of one or more days, select the third option and then select the desired number of days.

**5. Choose OK.**

If Monitoring is set to On, the expiration date of the item's last test results of system maintenance appears in the Expires box. When it is past time to perform the test of system maintenance again, the System Status indicator becomes red to alert you (If Monitoring is set to On).

**Configuring standards for Performance Verification or ValPro Qualification**

If Performance Verification or ValPro Qualification is available on your system, use the Configure Standards button in the System Status Overview dialog box to configure your standards, including specifying their expiration dates and other information. Follow these steps:

**1. Choose Configure System Status from the View menu.**

The System Status Overview dialog box appears.

**2. Click Performance Verification or ValPro Qualification.**

**3. Click the Configure Standards button.**

A dialog box lists the previously entered standards, if any.

**4. To add a new standard to the list, choose Add.**

In the dialog box that appears, select the desired standard from the drop-down list, enter its serial number, enter the date you are installing it and choose OK. The standard information appears in the list. The expiration date and replacement reminder date are based on the installation date and recommended lifetime of the standard.

**5. To change the information for a listed standard, select it and choose Update.**

In the dialog box that appears, change the information as desired (see the preceding step) and choose OK.

**6. To remove a listed standard, select it and choose Remove.**

**7. Choose OK.**

**Note** If a standard expires, the System Status indicator displays a red X. To see the expiration date, click the indicator and then click Performance Verification or ValPro Qualification. ▲

## **System Suitability**

The System Suitability features, if available for your system in System Performance Verification, let you check the suitability of your spectrometer for use in your particular application. You specify which of the following tests to perform, the spectral regions or frequencies to use, and the acceptance limits. The tests can be performed with your sample or automatically using a validation wheel, if installed. You do not need to set the parameters for the test when using the validation wheel.

**Note** To enable use of the wheel for the tests, use the Configure Bench button on the Configure tab in the Experiment Setup dialog box to select Validation Wheel Installed. ▲

**Noise** – Measures the rms and peak-to-peak noise in a baseline region of a “100% line” spectrum and compares the values with upper limits. This indicates the ability of the spectrometer to separate extremely weak spectral features from background noise. Your Trend Limit value is the maximum allowed absolute value of the slope of the baseline in the specified region.

**Throughput** – At up to three frequencies calculates the ratio of the measured % transmittance to that of a reference spectrum and compares the ratio with a lower limit. This indicates how much the spectrometer performance has changed since the reference spectrum was collected.

**Contamination** – In up to three spectral regions compares the measured absorbance of a “100% line” spectrum (data collected with no sample present) to verify that no unexpected (contaminant) peaks exceed the specified upper limit. Contaminant peaks may indicate the need to clean an ATR crystal or transmission cell.

**X-axis accuracy** – At up to three frequencies determines whether the measured peak frequency is within the specified tolerance. This verifies that the wavenumber value is as expected when a known sample is measured. This test and the next help ensure that the system will respond to test samples in a valid, predictable and meaningful manner. These tests are discussed in more detail below.

**Y-axis accuracy** – At up to three frequencies determines whether the measured peak absorbance intensity is within the specified tolerance. The test determines the top of the nearest peak and reports that value. This verifies that the intensity value is as expected when a known sample is measured.

To specify these tests, choose Configure System Status from the View menu to display the System Status Overview dialog box. Then click System Suitability and use the Configure button to set the test parameters for your application. See the recommendations for setting limits and tolerances later in this section.

You can use the Set Interval button to specify how often System Suitability checks must be performed. When it is past time to perform a new check, the System Status indicator becomes red. (For more information, click the indicator, click System Suitability in the System Status Overview dialog box and click the Explain Error button.)

To start a system suitability check at any time, click the System Status indicator near the top of the OMNIC window (or choose System Status or Configure System Status from the View menu), click System Suitability in the System Status Overview dialog box and then click the Run button. When the tests are finished, you can use the Report button to view or print a report showing the results. Printed results include a signature block.

### Setting appropriate limits and tolerances for System Suitability tests

We recommend not changing the tolerance values for the noise, throughput and contamination tests from their default values unless you have a clear understanding of the impact of the changes. The defaults were set to be appropriate for most applications. Since these tests are performed without a sample, sample-specific variations are not present. The X-axis and Y-axis accuracy tests require more consideration.

The regions for the contamination test were chosen based on the most common materials tested. If you change these regions, do not use spectral regions with bands overlapping common spectrometer features, such as atmospheric water vapor, unless you are interested in investigating the presence or absence of those materials. Typical background interferences are listed in the table below. Not all may apply to your configuration.

Spectral Range (wavenumbers)	Interference
5580-5500	NIR range, water vapor
3950-3500	Water vapor
2400-2270	Carbon dioxide
2670-1800	Diamond bands (diamond ATR)
2000-1290	Water vapor
700-400	Carbon dioxide
Below 650	Cut-off wavenumber for ZnSe (ATR)

In a purged system, you can use many of these ranges to check for the presence of atmospheric water or carbon dioxide. The fingerprint region is heavily affected by water vapor, but choose a check region in this range only with an understanding of the potential impact.

The limits and tolerances for the X-axis and Y-axis accuracy tests are discussed below.

### **X-axis and Y-axis accuracy tests**

If you are using the Automatic (internal validation wheel) option, the System Suitability test will collect the spectra from a 1.5 mil polystyrene sample and use three peaks in that sample data to measure the X-axis and Y-axis axis accuracy. You do not need to alter any values in the System Suitability Configuration dialog box when using this option, regardless of whether an additional accessory is in place; the ratio procedure in collecting the spectra will provide numbers within the tolerance range. This is in contrast to Performance Verification, which must be done with no accessory present. System Suitability using the internal validation wheel allows a modified version of the Performance Verification test with an accessory in place (but you must modify the limits on noise to reflect the impact of the accessory on throughput).

If you wish to use the Manual option and use a sample that you provide, you need to know the variability in both the sample and any other factors that would affect the measurements. You will need to obtain or make a “gold standard” reference sample of the test material, which will be used to define the test and to later check for compliance.

Considering first the X-axis, the tolerance setting of one wavenumber for X-axis accuracy is appropriate for most samples. You may enter the wavenumber (X) locations of up to three peaks present in your reference spectrum. You should choose peaks that are sharp and well isolated. Generally, the peak should be no more than 20 wavenumbers wide and not merged into another peak or be a shoulder on another peak.

To determine the tolerance for the Y-axis accuracy test, collect three to ten spectra from the reference in the sampling accessory. This should include samples covering the allowable variations in the reference; ideal reference samples are homogeneous and stable. If there is significant variation in the spectra, this will need to be accounted for in the tolerance values. Save these spectra and ensure sufficient availability of the reference material for future checking of System Suitability tests. This will remove one source of possible variation (sample to sample). If new material is used, it should be checked against the original to ensure consistent performance.



Use Find Peaks in the Analyze menu (or a manual process) to measure the peak heights of three (or fewer) peaks that you plan to use to determine Y-axis accuracy. Record the measured peak heights for the three to ten sample spectra. You can copy and paste the peak finding results directly into a spreadsheet to make this simple. Determine the average value and standard deviation of these measurements. Enter the average value for the peak location and the average value for the peak height into the appropriate column in the Y-axis Accuracy Test box. OMNIC will check for the peak closest to the set value, so there is no concern that the peak be at this exact location.

To set the tolerance, multiply the standard deviation for each peak by 3 and enter the result into the Tolerance column. Since the limit is plus or minus the tolerance, this represents a six-sigma range.

Before implementing your System Suitability test into an SOP, make sure that satisfactory pass/fail criteria have been set.

### **Setting the system suitability test parameters**

Follow these steps to set the System Suitability test parameters (if available for your system):

- 1. Choose Configure System Status from the View menu.**

The System Status Overview dialog box appears.

- 2. Click System Suitability and then click the Configure button.**

A dialog box appears.

- 3. If you want to use settings that you previously saved in an experiment file, use the Open button to open that file.**

- 4. Select the tests you want used.**

When you select a test, parameters for that test become available.

**5. Enter the limits and other needed information for each selected test.**

If a selected test has multiple sets of limits, select the ones you want used and adjust the limits as desired. You can click the Use Defaults button to set all the parameters to their default settings.

**6. The date that the current reference spectrum (if one exists) was collected appears above the Collect button. If you want to use a new reference spectrum, click the button to collect it.**

Follow the instructions that appear on the screen.

**7. If your system has a sample wheel that you want used for the tests, select Automatic in the Sampling box. Otherwise, select Manual.**

Enter the text you want used to prompt the operator to clear the sample compartment.

If you select Manual, also enter the text you want used to prompt the operator to insert the sample. The operator will be responsible for introducing the correct sample for the test when the specified prompt appears.

**8. To save your settings in the current experiment file, choose Save. To save the settings in a new file, use the Save As button.**

**9. When you are finished, choose OK.**

## **Checking instrument performance with Performance Verification**

The Performance Verification features, if available for your system in System Performance Verification, let you check the operation of the system to verify that it passes the following tests when performed using a TGS detector. These tests use traceable 1.5 mil polystyrene and NG11 samples mounted on an optional validation wheel. If the wheel is not installed and configured, Performance Verification is not available.

**Note** To enable use of the wheel for the tests, use the Configure Bench button on the Configure tab in the Experiment Setup dialog box to select Validation Wheel Installed. ▲

The 1.5 mil polystyrene is traceable to NIST SRM 1921a, and the NG11 glass is traceable to NPL Schott NG11. Analysis methods are based on ASTM E 1421-99 (2004) Standard Practice for Describing and Measuring Performance of Fourier Transform Mid-Infrared (FT-MIR) Spectrometers: Level Zero and Level One Tests. The test acceptance limits are set at our factory, with the exception of the wavelength accuracy test, which uses peak locations and acceptance limits published in the European Pharmacopeia, General Chapter 2.2.24, Absorption Spectrophotometry. Infrared NG11 intensity repeatability replaces the polystyrene photometry test, because it is deemed to be a more effective indication of linearity.

- Single-beam energy ratio – 9. Level one – 9.1 Energy Spectrum Test
- 100% transmittance noise level – 9. Level One – 9.2 One Hundred Percent Line Test
- 1.5 mil polystyrene wavelength accuracy – 9. Level One – 9.5 Polystyrene Tests - 9.5.1 Peak Positions
- NG11 intensity repeatability – 9. Level One – 9.5 Polystyrene Tests - 9.5.4 Photometry

To display the Performance Verification features, click the System Status indicator near the top of the OMNIC window (or choose System Status from the View menu) and click Performance Verification in the System Status Overview dialog box. The date of the last verification appears in the Last Performed box.

To perform a verification, click the Run button. When the tests are finished, you can use the Report button to view or print a report showing the results. Printed results include a signature block.

Use Configure System Status in the View menu to set up the Performance Verification parameters in the System Status Overview dialog box. You can use the Set Interval button to specify how often verifications must be performed. When it is past time to perform a new verification, the System Status indicator becomes red. (For more information, click the indicator, click Performance Verification in the System Status Overview dialog box and click the Explain Error button.) You can also set up a performance verification to run automatically at a scheduled time and configure the standards.

To view the latest verification results, click the Report button. You can then print the results, including the signature block, by clicking the Print button.

### **Setting up an automated performance verification**

If Performance Verification is available on your system, you can have a verification run automatically at a scheduled time using the internal validation wheel. You use the Task Scheduler wizard in Windows to set up the software for the verification.

*In Windows Vista:*

- 1. Click the Windows Start button, point to Control Panel, point to System And Maintenance, point to Administrative Tools and then choose Schedule Tasks.**
- 2. When you are asked to confirm launch of Microsoft MMC, choose Continue.**
- 3. Choose Create Basic Task in the Actions panel of Task Scheduler and then follow the wizard's instructions.**

When you are asked what action you want the task to perform, select Start A Program and choose Next. Then use the Browse button to locate and select the file named omnic32.exe. This file is typically in C:\Program Files\OMNIC; the specific location depends on where you installed OMNIC.

In the Add Arguments (optional) text box enter the following:

-C“PerfVerifyTest; Select All; DeleteSelectedSpectra; Exit”

Type this text exactly as it appears above, including the quotation marks.

When the Open The Properties Dialog For This Task When I Click Finish check box appears, select it and then choose Finish. A dialog box appears. Select Run Whether User Is Logged On Or Not on the General tab. Set the parameters on the other tabs as desired and then choose OK.

*In Windows XP:*

- 1. Click the Windows Start button, point to All Programs, point to Accessories, point to System Tools and then choose Scheduled Tasks.**
- 2. Double-click the Add Scheduled Task icon and then follow the wizard's instructions.**

When you are prompted to select a program to run, use the Browse button to locate and select the file named omnic32.exe. This file is typically in C:\Program Files\OMNIC; the specific location depends on where you installed OMNIC.

When the Open Advanced Properties For This Task When I Finish check box appears, select it and then choose Finish. A dialog box appears. At the end of the text in the Run text box on the Task tab, type a single space followed by:

-C“PerfVerifyTest; Select All; DeleteSelectedSpectra; Exit”

Type this text exactly as it appears above, including the quotation marks.

Set the parameters on the other tabs as desired and then choose OK.

## Checking instrument performance with ValPro Qualification

If you have installed ValPro Qualification software, the ValPro Qualification features are available in System Performance Verification. They let you check the performance of your instrument with an expanded test suite by comparing the current qualification results with those obtained in the past to verify that the system is working consistently over time.

**Note** To set options for performing qualifications, choose ValPro Qualification from the Analyze menu and click the Options button in the ValPro Qualification window. Use the Qualification Tests tab to specify the tests to include. Use the SPV Monitoring tab to select the methods to be monitored by System Performance Verification when ValPro Qualification monitoring is enabled. (Click the Help button for instructions or to access information about the qualification tests in the ValPro Qualification Help system.) You can also set some options by choosing Configure System Status from the View menu, clicking ValPro Qualification and then using the buttons that appear to the right. ▲

You can start a qualification at any time by clicking the Run button and following the instructions that appear on the screen. When the tests are finished, you can use the Report button to view or print a report showing the results. Printed results include a signature block.

You can use the Set Interval button to specify how often ValPro Qualification tests must be performed. When it is past time to perform a new test, the System Status indicator becomes red. (For more information, click the indicator, click ValPro Qualification in the System Status Overview dialog box and click the Explain Error button.)

**Note** If OMNIC does not display the last date the a qualification was performed, make sure you have installed ValPro Qualification version 2.2 or greater. ▲

## Using Scheduled Maintenance

The Scheduled Maintenance feature of System Performance Verification lets you set up scheduling of system maintenance and be informed when maintenance needs to be performed. The required maintenance tasks depend on the system model. To enable this feature:

### 1. Choose Configure System Status from the View menu.

The System Status Overview dialog box appears.

**2. Click Scheduled Maintenance.****3. Set Monitoring to On.****4. Choose OK.**

Use the Set Interval button to specify how often system maintenance should be performed. When the maintenance expiration is within the period you specify with the Configure button (explained below), the System Status indicator becomes yellow and a message informs you of the pending expiration. This provides a reminder to schedule a service visit. When it is past time to perform system maintenance, the System Status indicator becomes red. (For more information, click the indicator, click Scheduled Maintenance in the System Status Overview dialog box and click the Explain Error button.)

When maintenance is performed, use the Configure button to enter the current date in the Scheduled Maintenance dialog box. The maintenance expiration specified with the Set Interval button will be based on this date. Also enter the number of days before the specified expiration date that you want to be reminded to schedule a service visit.

**Viewing the results of spectral quality checks**

The Last Spectral Quality Result feature of System Performance Verification lets you view the results of the last spectral quality checks performed on collected data. (To use these checks, select Use Spectral Quality Checks on the Quality tab of the Experiment Setup dialog box.)

If spectral quality checks have been used, the Display button appears when you click Last Spectral Quality Result in the System Status Overview dialog box. Click the button to see the check results, displayed in the Collect Status dialog box. (This dialog box also appears when you click the View Collect Status button following data collection.) If a check failed, an Explain button appears in the dialog box; click it to see information about correcting the problem. Keep in mind that the displayed results are for the last spectrum collected with spectral quality checks being used, not necessarily the last spectrum you collected.

**Note** The Last Spectral Quality Result features do not affect the appearance of the System Status indicator near the top of the OMNIC window. A failure of a spectral quality check does not change that indicator from green to red, for example. ▲

## Using Experiment Setup

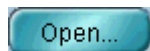
Use Experiment Setup in the Collect menu to set the parameters that control how spectra are collected—including which beam path and accessory are used—and how collected spectra are checked for quality. You can also use the command to perform diagnostic checks of the spectrometer and to align it.

After you set the parameters for a particular type of experiment, you can save the settings in a file named for that experiment type. When you want to perform a similar experiment later, you can quickly reset the parameters to the required settings by simply opening the appropriate experiment file. (When you install a Smart Accessory, the appropriate experiment is automatically selected for you.) We recommend setting up and saving an experiment for each of your commonly used applications.

**Note** Your OMNIC software includes several example experiment files. These experiments contain parameter settings appropriate for use with various OMNIC tutorials and for collecting spectra using different applications. See “Using the provided example experiments” for more information. If you have changed the parameter settings in one of these experiments, you can quickly restore the parameters to their default settings before using the experiment. See “Restoring the default settings” for details. ▲

When you choose Experiment Setup from the Collect menu, the Experiment Setup dialog box displays any one of several sets of features. (If you have OMNIC Atlas 7.0 or greater, the Mapping tab is included. See the *OMNIC Atlas User's Guide* for more information. If you have OMNIC Series 7.3 or greater, the Series tab is included. See the OMNIC Series Help system for more information.) Each set is contained on a tab whose name is always visible at the top of the dialog box. To display a set of features, click the appropriate tab. The features are brought to the front.





To use the parameter settings contained in an experiment file, use the *Open button*. You can open the example experiment files provided with OMNIC or files you have set up and saved (explained below). When you select a file in the Open Experiment dialog box, its title and description appear near the bottom of the dialog box, making it easier to find an appropriate experiment.

**Note** You can open a parameter file from an early version of OMNIC (3.0 or earlier) by first selecting the Parameter Files file type (\*.PRM) in the Open Experiment dialog box. ▲

**Note** When you are not using Experiment Setup, you can select a saved experiment for use from the Experiment drop-down list box near the top of the OMNIC window. (The experiments available in the list box are those in the current experiment directory that have been opened by using Experiment Setup or by installing a Smart Accessory.) See “Selecting an experiment” for more information.

The experiment you select also sets the parameters in the Library Setup dialog box (except for those on the Library Directories tab) and the parameters in the QCheck Setup dialog box. See “Setting up a spectral search or QC comparison” in the “Analyze” chapter for complete information about Library Setup. See “Setting up a QCheck comparison” in that chapter for information about QCheck Setup. ▲

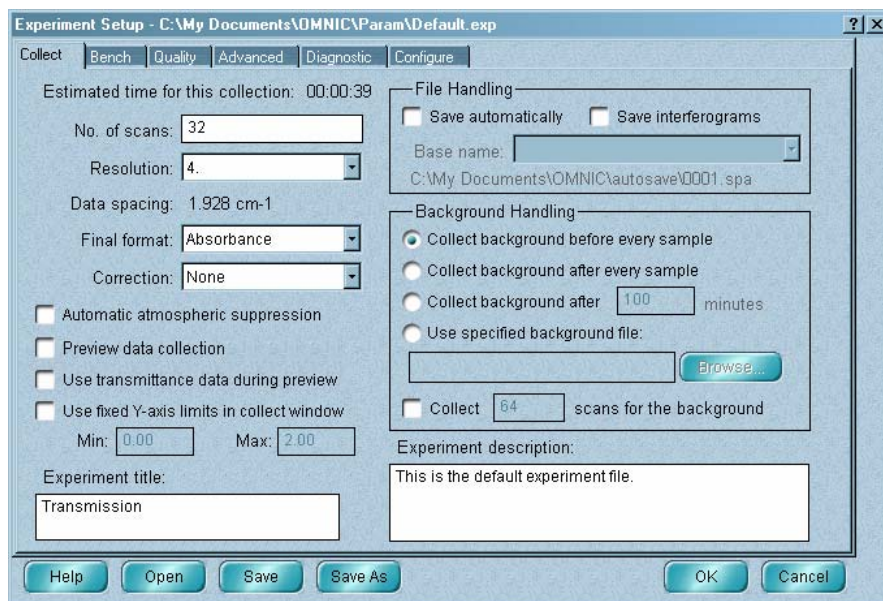


After you have set the parameters, you can save them in an experiment file by using the Save button (to use the current experiment filename) or Save As button (to use a different filename). If you want the experiment you are saving to be the default experiment, use the Save As button and turn on the Set As Default Experiment check box in the Save Experiment As dialog box. The next time you log into OMNIC, that experiment will be selected automatically. If you want the experiment saved so that it can be opened later but not changed and saved with the changes, turn on the Read Only check box in the Save Experiment As dialog box.

To delete an experiment file, use Delete Files in the File menu. See “Deleting files” in the “File” chapter for details.

## Collect parameters

The Collect tab contains parameters for specifying the items shown and described in the following illustration and table.



### To specify or do this...

### Set this parameter...

See how long the data collection will take. The time is displayed in hours:minutes:seconds. The total collection time is determined by the number of scans collected and the resolution.

Estimated Time For This Collection (if available for your spectrometer)

The number of scans to collect.

Number Of Scans

The spectral resolution of the data.

Resolution

See the distance between adjacent data points in the collected spectrum in wavenumbers. The data spacing is determined by the settings of resolution and zero filling (set on the Advanced tab).

Data Spacing

The Y-axis format of collected data.

Final Format

The correction type to use.

Correction

Automatically suppress the effects of water vapor and carbon dioxide.

Automatic Atmospheric Suppression

To specify or do this...	Set this parameter...
Check the performance of the spectrometer at the start of data collection.	Preview Data Collection
Display preview data in % transmittance with fixed Y-axis limits.	Use Transmittance Data During Preview
The Y-axis display limits for the Collect Sample and Collect Background windows.	Use Fixed Y-Axis Limits In Collect Window
The title of the experiment.	Experiment Title
Save spectra automatically.	Save Automatically
Save interferograms with spectra.	Save Interferograms
The base name for saving spectra automatically.	Base Name
Whether and when to collect a background spectrum or use a stored background, and how many background scans to collect.	Background Handling
A description of the experiment.	Experiment Description

### Specifying the number of scans

No. of scans:

Number Of Scans on the Collect tab determines how many scans are performed during a sample or background data collection. If you perform more than one scan, the system averages all of them.

**Note** You can specify a different number of background scans by selecting Collect \_\_\_ Scans For The Background in the Background Handling box. When that option is selected, the setting of Number Of Scans affects only sample data collection. See “Background handling” for more information. ▲

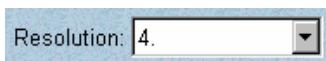
The number of scans, along with the resolution and optical velocity, affects the total collection time. For a given resolution, increasing the number of scans increases the total collection time.

Increasing the number of scans reduces the noise level of the data (increases the signal-to-noise ratio) and increases the sensitivity; that is, the ability to distinguish small peaks from noise. However, if you have already collected a large number of scans, it will take many more scans to achieve a significant increase in sensitivity.

Optimize the Number Of Scans setting whenever you analyze a new type of sample or use a new sampling technique or accessory. If you're not sure how long to scan, start by collecting 16 scans and then measure the signal-to-noise ratio. This will give an indication of how many scans to collect for the desired results.

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

### Specifying the resolution



The Resolution parameter on the Collect tab sets the spectral resolution of the data you collect. It determines how close two peaks can be and still be identified as separate peaks.

The smaller the resolution value, the higher (better) is the resolution. Increase the resolution (use a smaller value) when you need to distinguish narrower bands. Smaller values can produce narrower bands because the points in the spectrum are closer together.

The resolution value, along with the number of scans and optical velocity, affects the total collection time. For any given number of scans, increasing the resolution (using a smaller value) increases the total collection time.

Set the resolution only as high as needed to differentiate peaks of interest and give good search results. Setting the resolution higher will not provide more information and can result in increased noise. Also, the higher the resolution, the longer it takes to collect the data and the more disk space that is required to save the data.

Typically resolutions of 8 or 4 wavenumbers are used for solid and liquid samples. Gas samples normally require a resolution of 2 wavenumbers or preferably 1.0 or 0.5 wavenumber.

To optimize resolution, start by scanning the sample at a low resolution setting; 4 wavenumbers, for example. Then increase the resolution and scan the sample again. Overlay the spectra so you can compare their quality. Repeat this procedure until the spectra show little or no corresponding increase in spectral information. The lower of the last two resolutions is the preferred setting.

When the resolution is 2 wavenumbers or better (lower setting of Resolution), use the appropriate aperture setting. A small aperture restricts the infrared beam and thus limits the distortion that can occur at high resolutions when a large aperture is used.

Collect your sample and background spectra using the same resolution.

### Selecting the final format

Final format: Absorbance

Final Format on the Collect tab determines the units for the collected data. The following table shows the available format settings and the units used.

Setting	X-Axis Units	Y-Axis Units
Interferogram	data points	volt
SingleBeam	wavenumber	arbitrary units
%Transmittance	wavenumber	% transmittance
Absorbance	wavenumber	absorbance units
Kubelka-Munk	wavenumber	Kubelka-Munk units
Photoacoustic	wavenumber	photoacoustic units
%Reflectance	wavenumber	% reflectance units
Log(1/R)	wavenumber	log (1/R) units

To convert collected data to other Y-axis units, use Absorbance, % Transmittance or Other Conversions in the Process menu.

## Selecting a correction type

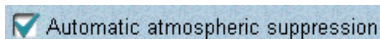


Use the Correction parameter on the Collect tab to specify the type of correction to use when collected spectra are processed. The following types are available.

- None (no correction)
- Kramers-Kronig
- ATR
- H<sub>2</sub>O
- CO<sub>2</sub>
- H<sub>2</sub>O And CO<sub>2</sub>

See “Using Other Corrections” in the “Process” chapter for descriptions of these correction types.

## Automatically suppressing atmospheric effects



Select Automatic Atmospheric Suppression, if available on the Collect tab, if you want the effects of water vapor and carbon dioxide on collected spectra to be automatically suppressed through the use of a quantitative model.

If you find that this feature does not adequately suppress the effects of water vapor and carbon dioxide absorptions in the sample spectra you collect, you can use the features in the Atmospheric Suppression box in the Process options (available through Options in the Edit menu) to improve your results. See “Specifying an additional reference for atmospheric suppression” in the “Edit” chapter for details.

This feature suppresses the effects of water vapor in the spectral range from 4000 to 400 wavenumbers. It suppresses the effects of carbon dioxide in the range from 4000 to 720 wavenumbers.

This feature is useful when you infrequently collect background spectra or when atmospheric conditions change rapidly. In these cases significant differences between the atmospheric absorptions present in background and sample spectra are likely.

Do *not* use this feature if you collect a background before each sample spectrum or when atmospheric conditions change very slowly. In these cases it is unlikely that the atmospheric absorptions in your spectra have changed significantly. It is better to ratio the absorptions out (by ratioing the sample single-beam spectrum against the background single-beam spectrum).

When deciding whether to use this feature, keep in mind that a tradeoff exists: The benefit, removing gross atmospheric signals from the spectral data, is offset to some extent by the introduction of minor artifacts.

These artifacts are due to a combination of factors. One is the natural bias from statistics; when absorptions are caused by unknown components, this is unavoidable. The other factor is the fact that there may be atmospheric signal that is not described in the set of standards used to develop the quantitative model. You can improve this by adding your own standards. (See the explanation above.)

**Note** You can also use the water and carbon dioxide corrections available through Corrections on the Collect tab or Other Corrections in the Process menu to correct spectra for absorptions due to water vapor and carbon dioxide. However, we recommend using Automatic Atmospheric Suppression instead, unless you find that the humidity in your facility is too high for it to work effectively. ▲

### Checking spectrometer performance at the start of data collection

Preview data collection

Select Preview Data Collection on the Collect tab if you want to collect and view (but not save) preliminary data before the start of a sample or background data collection. This lets you verify that your experimental conditions are correct before collecting the spectrum.

If you want the preliminary data displayed in % transmittance with a fixed Y-axis scale, select Use Transmittance Data During Preview. This can provide an improved view of the data.

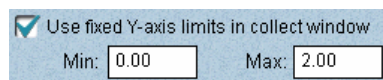
If you choose Collect Sample or Collect Background from the Collect menu when the parameter is on, the system continuously collects and displays data in the specified final format until you click the Start Collection button.

### Displaying preview data in % transmittance with a fixed Y scale

Use transmittance data during preview

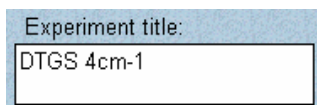
If you have selected Preview Data Collection on the Collect tab, select Use Transmittance Data During Preview on the Bench tab if you want the preliminary data displayed in % transmittance, with a Y-axis range of -5 %T to 105 %T. This can provide an improved view of the preliminary data.

## Specifying the Y-axis display limits for data collection



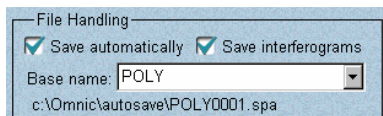
Normally spectral data is displayed full scale during collection. You can specify particular Y-axis display limits by selecting Use Fixed Y-Axis Limits In Collect Window on the Collect tab and typing the desired limits in the Min and Max text boxes. This can help you see small peaks that would otherwise appear very small when a large peak is displayed full scale. It is especially useful when you are previewing data collection. See “Checking spectrometer performance at the start of data collection” for more information.

## Titling the experiment



Type a title for the experiment in the Experiment Title box on the Collect tab. When you save the experiment and open or select it later, the title will appear in the box. (The experiment title also appears in the dialog box that displays the results of the spectral quality checks made during data collection and in the EXPERIMENT INFORMATION section in the Collection And Processing Information window for a collected spectrum.) The saved experiment will be available for selection in the Experiment drop-down list box (if available) near the top of the OMNIC window.

## File handling



The options in the File Handling box on the Collect tab let you save collected spectra automatically.

Turn on Save Automatically to save spectra immediately after collection. (Final Format determines the Y-axis unit used.) The files are named with a four-character base name plus a sequence number with up to four digits, followed by an extension. Type a name in the Base Name box or select a base name from the drop-down list box. Use a descriptive base name for each group of samples so you can find them easily later. After you specify a base name and then perform another operation, the path that will be used when the spectra are saved appears below the Base Name box.

The extension and sequence number are assigned by the software, with the extension .SPA used for sample and background spectra. The sequence number is increased by one each time you collect a spectrum. For example, if the base name is POLY, the first sample will be named POLY0001.SPA, the second POLY0002.SPA and so on. If you use a previously used base name, the sequence numbers for new files will begin where the previous numbers left off.



The spectra are saved in the directory indicated by the path below the Base Name box. You can change this path by using the File options (available through Options in the Edit menu; see “Specifying directories” in the “Edit” chapter for details).

Turn on Save Interferograms if you want to include the associated background and sample interferograms when a spectrum is saved. The interferograms will be saved in the same file as the spectrum. The interferograms will be included whether you are saving spectra automatically or saving them by using Save in the File menu.

Saving interferogram data lets you reprocess in case you want to restore the original data. When you reprocess the spectrum, you can use a different background or change some of the parameter settings used for the transformation.

Save interferograms if archiving or reprocessing of data is important to your work. An interferogram is raw data that can be processed. By saving interferograms, you can always recreate the original spectrum (in the same state as when it was collected). This gives you a way to eliminate baseline corrections or other corrections and changes you have made to the data.

**Note** The Save Interferograms parameter on the Collect tab does not affect series data collection. If you have OMNIC Series, use Save Interferograms on the Series tab to specify whether to save interferograms for your series experiments. ▲

### Background handling

Background Handling

Collect background before every sample

Collect background after every sample

Collect background after 100 minutes

Use specified background file:

Collect 64 scans for the background

The options in the Background Handling box on the Collect tab let you specify when to collect a background or select a stored background for ratioing sample spectra you collect.

Select Collect Background Before Every Sample if you want to collect a background spectrum before each sample spectrum. Select Collect Background After Every Sample if you want to collect a background spectrum after each sample spectrum.

The Collect Background After \_\_\_ Minutes option prompts you to collect a background after the specified number of minutes. This option is usually the best choice for most applications. If you select it, type the desired number of minutes in the box to the left of Minutes. You can use the Collect options (available through Options in the Edit menu) to specify how you will be prompted. (You will be prompted to collect a background the very first time you collect a sample spectrum.)

To use a stored background, select Use Specified Background File. Type the name of the background file you want to use in the box next to Browse or choose Browse and select a background using the dialog box that appears. This background will be used when collected sample spectra are ratioed. You will not be able to collect a new background while this option is selected.

**Note** To store a background on a disk manually, use Collect Background in the Collect menu and then save the background spectrum using Save in the File menu. See “Collecting a background spectrum” in this chapter and “Saving a spectrum” in the “File” chapter for more information. ▲

If the selected background is not adequate for the sample spectrum you are collecting (because of a difference in resolution or data spacing), you will be prompted to collect a new background.

For demanding applications, you can obtain the best results by collecting the background just before or just after each spectrum.

**Note** If you are collecting step-scan data, do not use Collect Background Before Every Spectrum or Collect Background After Every Spectrum. ▲

Typically the same number of scans are collected for both background and sample spectra. You can collect a different number of background scans by selecting Collect \_\_\_ Scans For The Background and typing the desired number in the text box. When this option is selected, the Number Of Scans parameter affects only sample data collection.

### Entering an experiment description

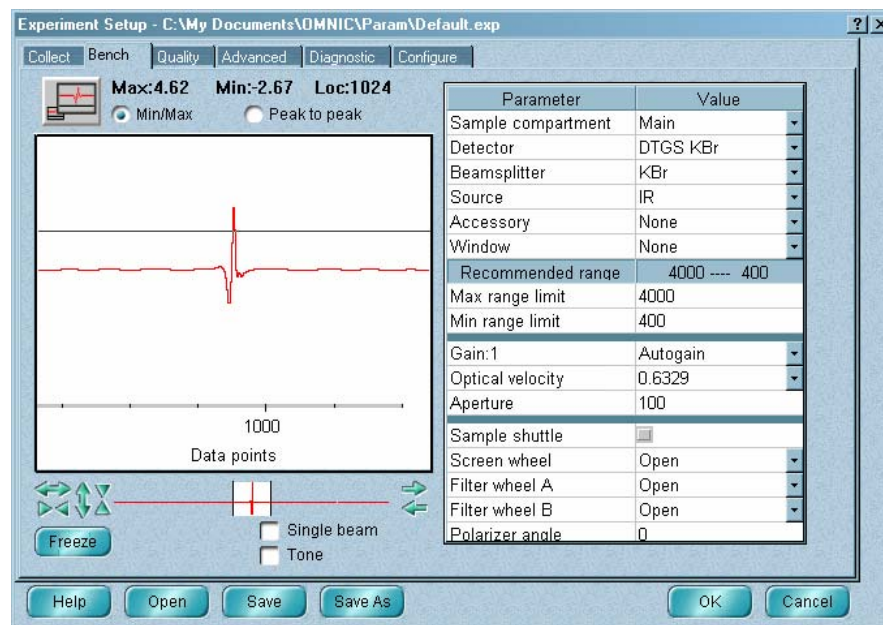
Experiment description:

This is the default experiment file.

Type a description of the experiment in the Experiment Description box. When you save the experiment and open or select it later, the description will appear in the box, serving as a reminder of the experiment’s purpose or as a record of other useful information.

## Bench features

The Bench tab contains the parameters and other features shown and described in the following illustration and table. (Depending on your system hardware, some features may not appear on the tab.)

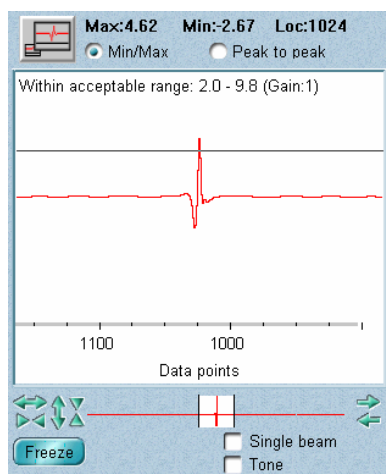


To specify or do this...	Use this feature...
Interact with the live display of the detector signal.	Live display
How to express the interferogram peak amplitude.	Min/Max or Peak To Peak
Display the signal as a single-beam spectrum.	Single Beam
Produce a tone during each scan.	Tone
Freeze an image of the detector signal in the live display.	Freeze button
The sample compartment to use.	Sample Compartment
The detector type.	Detector
The beamsplitter type.	Beamsplitter
The source type.	Source
The accessory that will be used for data collection.	Accessory

To specify or do this...	Use this feature...
The material that an accessory window is made of.	Window
The spectral range to save.	Max Range Limit and Min Range Limit
The detector signal gain.	Gain
The optical velocity.	Optical Velocity
The aperture size.	Aperture
Use a sample shuttle.	Sample Shuttle
Control the optional filter wheel.	Filter Wheel A and Filter Wheel B
Control the optional polarizer.	Polarizer Angle
Control the optional energy screen wheel.	Screen Wheel

At the left side of the Bench tab is a live display of the detector signal. If your spectrometer requires manual alignment, watch the live display while making the appropriate adjustments on it. The goal of manual alignment is to increase the Max value above the live display to its highest possible level. See the manual that came with the spectrometer for instructions on making the adjustments. You can also watch the live display while manually aligning an accessory.

### Using the live display



At the left side of the Bench tab is a live display of the detector signal (see the example at the left), which normally appears as an interferogram. The interferogram peak indicates the intensity of the signal. In general, a greater signal intensity will result in better, less noisy spectra. If you are manually aligning an accessory, watch the live display while you make adjustments to increase the intensity.

If Min/Max is turned on, the maximum (Max) and minimum (Min) signal intensities are shown above the live display along with the data point location (Loc) of the interferogram peak (see the example at the left).

If Peak To Peak is turned on, the peak-to-peak intensity of the signal is shown instead.

Here is an example:

**Peak to Peak:9.26    Loc:1024**

The peak-to-peak intensity is the sum of the absolute values of the maximum and minimum signal intensities. Displaying the signal intensity as a peak-to-peak value gives a clearer indication of the overall interferogram size, since it is one value instead of two values that need to be combined.

A readout near the top of the live display states whether the interferogram peak amplitude is within the acceptable range specified by the Peak Amplitude Within Range check on the Quality tab, if that check is being used. See “Checking the interferogram amplitude” for more information.

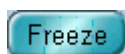
**Note** For the purposes of this check the interferogram amplitude is automatically normalized to a gain value of 1 to compensate for changes that can occur at different actual gain settings. ▲

When you manually align an accessory or change experiment parameters, you can visually determine whether the signal intensity has increased or decreased. To do this, click the tip of the largest interferogram peak (or the top of the single-beam spectrum) before aligning the accessory or making parameter changes. A horizontal line passes through the clicked point. Then make an alignment adjustment or parameter change and compare the new intensity with the line.

You can adjust your view of the live data by using the view finder below the live display. It works the same as the view finder in a spectral window. See “View finder” in the “About the Display” chapter if you need help.



If you need to see the live display from a distance (for example, when you are aligning an external accessory), you can enlarge the display by clicking the Enlarge button above the live display. To return to the normal live display, click the Enlarge button again.



To freeze an image of the detector signal in the live display, click the Freeze button. This lets you see changes by comparing the current signal with the frozen image. If you click the button again, a frozen image of the current signal replaces the old frozen image.



If you want to see an indication of the water vapor and carbon dioxide levels in the spectrometer or the frequency cutoffs of the system, turn on Single Beam to display the detector signal as a single-beam spectrum. Water absorptions occur at 3,800 and 1,600 wavenumbers, and carbon dioxide absorptions occur at 2,350 and 668 wavenumbers. The frequency cutoffs are the limits of the X-axis.

**Note** The location readout (above the live display) and the interferogram amplitude check readout (near the top of the live display) do not appear when Single Beam is on. ▲

If you want a tone produced during each scan of the interferometer, turn on the Tone option. At a given setting of the Gain parameter, the pitch of the tone rises as the signal intensity increases. If you increase the setting of Gain, the pitch of the tone rises. The Tone feature is useful when you are manually aligning a spectrometer or accessory and cannot see the display monitor.

### Specifying the sample location



Use Sample Compartment on the Bench tab to specify the location of your sample. The setting determines the path of the infrared beam through the spectrometer and any accessory. The available settings (see the following table) depend on the configuration of the spectrometer and accessories.

Setting	Use this setting if...
Main	The sample is in the sample compartment of the spectrometer.
GC Interface Right	You are performing a series experiment with the GC interface installed on the right side of the spectrometer.
GC Interface Left	You are performing a series experiment with the GC interface installed on the left side of the spectrometer.
Right $\mu$ Scope; %T	You are performing a transmission experiment using a microscope installed to the right of the spectrometer.
Right $\mu$ Scope; %R	You are performing a reflection experiment using a microscope installed to the right of the spectrometer.

Setting	Use this setting if...
Left $\mu$ Scope; %T	You are performing a transmission experiment using a microscope installed to the left of the spectrometer.
Left $\mu$ Scope; %R	You are performing a reflection experiment using a microscope installed to the left of the spectrometer.
Left AEM	The sample is in the sample compartment of an AEM installed to the left of the spectrometer.
Right AEM	The sample is in the sample compartment of an AEM installed to the right of the spectrometer.
Seaport	The sample is in an external accessory to which the infrared beam is directed by the optional Seaport optics.
Right TOM	You are using a TOM kit installed to the right of the spectrometer.
Left TOM	You are using a TOM kit installed to the left of the spectrometer.

### Specifying the detector type

Detector DTGS KBr

Use the Detector parameter on the Bench tab to specify the type of detector you will use for data collection. The available choices depend on the spectrometer and sample compartment you are using.

Typically MCT detectors are used rather than DTGS detectors if the amount of infrared energy reaching the detector is small (and liquid nitrogen is available for cooling the MCT detector dewar). MCT detectors are also commonly used when a high optical velocity is required; for example, in series experiments.

### Specifying the beamsplitter type

Beamsplitter KBr

The Beamsplitter parameter specifies the type of beamsplitter you will use for data collection. The available types depend on your spectrometer. If the spectrometer has automatic beamsplitter recognition, the type is set automatically and cannot be changed. Use the beamsplitter type that is appropriate for the spectral range of your experiment.

### Specifying the source type

Source	IR
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Use the Source parameter on the Bench tab to specify the type of source you will use for data collection. The available types depend on your spectrometer.

The IR - Rest setting, if available, enables Rest mode, helping to extend the life of the source.

The IR - Turbo setting, if available, places the source into Turbo mode, increasing the energy output. (The improvement in output increases with increasing wavenumber value.) This is useful when you are analyzing a sample, such as a thick film, that requires greater infrared energy.

**Note** Due to saturation and linearity effects, you should handle the extra energy from Turbo mode appropriately when using a sensitive detector like an MCT-A or MCT-B. Highly absorbing samples can benefit from Turbo mode, even with sensitive detectors, but use care during background collections: You may need to use an energy screen or an appropriate aperture setting to prevent detector saturation. ▲

Use a source type that is appropriate for the spectral range of your experiment.

### Specifying the accessory

Accessory	Smart Performer
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Use the Accessory parameter, if available on the Bench tab, to specify the type of accessory you will use to collect spectra. If you will not be using an accessory, select None.

If you select a Smart Accessory and then save the experiment, the experiment will be available for your selection in the window that appears the next time you install that Smart Accessory. If you wish, you can make several different experiments available for the same Smart Accessory by setting them up using Experiment Setup and saving them with descriptive titles.

**Note** When you install a Smart Accessory that has just one experiment associated with it (normally an experiment that was included with OMNIC), the system automatically sets up the software for it; you don't need to select an experiment or set the Accessory parameter. ▲



Select Custom Accessory if you are using an optional “Custom Accessory” Smart baseplate on which you have mounted an accessory you have built or purchased from another manufacturer. Just as with a standard Smart Accessory, any experiments you set up and save with Custom Accessory selected will be available the next time you install the baseplate.

The setting of Accessory affects the limits and other attributes used when the selected quality checks are performed during data collection. See “Quality checks” for more information.

### Specifying the window material

Window	kBr	▼
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Use Window on the Bench tab to specify the material of the window of the accessory used to collect spectra. If you will not be using an accessory with a window, select None. The setting affects the quality checks performed during data collection and the default spectral range.

**Note** The setting is saved in the collection and processing information for the spectrum. ▲

### Specifying the spectral range

Recommended range	4000 ---- 400
Max range limit	4000.00
Min range limit	400.00

Use the Max Range Limit and Min Range Limit parameters on the Bench tab dialog box to specify the frequency range (X-axis limits in wavenumbers) of the collected data to be saved on the hard disk. Data outside the specified range will not be saved.

To enter the upper limit of the range, double-click the table cell to the right of Max Range Limit. Then type a value or click the up and down arrow buttons to the right of the value.

To enter the lower limit of the range, double-click the table cell to the right of Min Range Limit. Then type a value or click the up and down arrow buttons to the right of the value.

If you don't enter a limit, the default value will be used. The widest limits recommended for the current configuration of the spectrometer are shown to the right of Recommended Range. These limits depend on which source, beamsplitter and detector are installed.

Use a spectral range that is appropriate for the detector. Data that fall outside the range will be lost when the spectrum is saved. (If you are saving interferograms, you can recover the lost data.)

To save disk space, set the range to include only the regions that are important to your experiment.

### Setting the gain

Gain:1	1.0	▼
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The Gain parameter on the Bench tab determines how much the detector signal is amplified electronically, making it larger relative to the level of electronic noise. Amplifying the signal is helpful when the signal is weak, such as when you use some sampling accessories. For example, ATR and diffuse reflection accessories typically use a Gain setting of 2 or 4. Select the desired setting from the drop-down list box at the right end of the Gain row.

You can let OMNIC automatically adjust the gain to maximize the signal by setting Gain to Autogain. For spectrometers other than Mattson and IR Series models, we recommend using this setting to ensure the best spectral quality for experiments not involving quantitative analysis.

**Note** Set Gain to 1 before performing an automatic alignment. ▲

The actual gain value appears immediately to the right of Gain.

**Note** The Gain parameter does not affect detectors used with the optional detector interface kit. ▲

### Specifying the optical velocity

Velocity	0.6329	▼
----------	--------	---

The Optical Velocity parameter on the Bench tab determines the optical velocity (a value that is twice the velocity of the moving mirror in the interferometer). The default value is determined by the detector type and is set when you specify a detector with the Detector parameter. Select the desired setting from the drop-down list box at the right end of the Optical Velocity row.

Using a faster velocity lets you collect more scans in a given amount of time; however, using a velocity that is faster than the default setting will produce a noisier signal.

If you are using a sampling accessory with very low throughput, you may find that you can increase the signal intensity to an adequate level by using a slower velocity. The results will depend on the detector you are using.

Using a slower velocity increases the time required for an individual scan, but that does not mean the total measurement time needs to be longer. The stronger signal obtained (with some detectors) at the slower velocity can allow you to collect fewer scans, resulting in a shorter measurement time and better quality spectra.

**Note** While a wide range of moving mirror velocities is available, some velocity settings cannot be used for collecting data at certain combinations of spectral range and resolution (and sample spacing for a Nicolet 8700, Nicolet Nexus 870 or Magna-IR 860). See the documentation that came with your spectrometer for details. ▲

For information about setting the optical velocity for specific spectrometer models, find “optical velocity” in the OMNIC Help system Index and go to the “Specifying the optical velocity” topic.

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

### Setting the aperture size

Aperture	100
----------	-----

Use the Aperture parameter on the Bench tab to set the size of the aperture opening. The aperture is a variable-diameter opening which controls the intensity of the infrared radiation that reaches the sample.

**Note** On systems with a fixed-diameter aperture, Aperture is not available or has no effect on the aperture opening. The rest of this topic applies only to systems with an adjustable aperture. ▲

Using an aperture provides the following advantages:

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

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

DTGS detectors can accommodate most of the energy from the source, which means you should use a large aperture size. Detectors that require cooling with liquid nitrogen are very sensitive and require a small aperture size or the use of an energy screen (see your system manual and Installing Hardware in the Help menu for more information on using energy screens).

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

Detector	Setting
DTGS	100 (30 for Mattson systems with an adjustable aperture)
MCT-A, MCT-B, InSb, PbSe, InGaAs, Si	32 (10 for Nicolet 380; Nicolet Avatar or Nicolet Protégé system with half-wavenumber option; Mattson systems with adjustable aperture)

The following table shows the allowed values for different spectrometer models. The actual size of the opening is determined by the installed aperture.

Model	Allowed Values
Nicolet iS10	High Resolution, Medium Resolution, Open

Model	Allowed Values
Nicolet 4700; Nicolet 5700; Nicolet 6700; Nicolet 8700; Nicolet Nexus with adjustable aperture; Magna-IR	0 (minimum size) to 150 (maximum size)
(For these systems the Aperture setting determines the <i>area</i> of the aperture opening. Doubling the setting approximately doubles the area.)	
Nicolet 380; Nicolet Avatar; Nicolet Protégé with half-wavenumber option	10, 100

**Note** When collecting spectra at a resolution of 2 wavenumbers or higher (lower setting of the Resolution parameter), be sure to use the aperture setting shown in the table above. A small aperture restricts the infrared beam and thus limits the band distortion that can occur at high resolutions when a large aperture is used. ▲

### Using a sample shuttle

 Sample shuttle 

Select Sample Shuttle on the Bench tab if you are using a sample shuttle in the sample compartment of your spectrometer or sampling accessory. If the option is selected, the sample shuttle will move to the appropriate position—sample or background—when you collect a spectrum. Be sure to place the sample in the appropriate slot of the shuttle.

### Controlling the energy screen wheel

Use the Screen Wheel parameter, if available on the Bench tab, to control the optional energy screen wheel in a Nicolet 4700, Nicolet 5700, Nicolet 6700 or Nicolet 8700 spectrometer. The wheel lets you automatically insert an energy screen into the beam path to block out a portion of the energy at all frequencies.

The wheel has four positions: an open position for collecting spectra without a screen in the beam path, and three positions that each hold a screen that passes a different percentage of the infrared energy. See your spectrometer documentation for more information about the screens installed in the wheel.

To specify the wheel position to use, select the desired setting from the drop-down list box at the right end of the Screen Wheel row. The settings indicate the percentage of the energy that passes through the screen.

You can change the descriptions that appear in the drop-down list box by using the Screen Wheel features on the Configure tab. See “Specifying the energy screens in the energy screen wheel” for more information.

### Controlling the filter wheel

Filter wheel A	Open	▼
Filter wheel B	Open	▼

Use Filter Wheel A and Filter Wheel B, if available on the Bench tab, to control the optional filter wheel accessory. The two wheels of the accessory let you automatically insert up to two optical filters into the beam path to control the spectral range of the infrared beam. For example, you can use a single high pass filter to eliminate frequencies at one end of the range. You can also use a combination of a high pass filter on one wheel and a low pass filter on the other to limit the range in other ways.

Each wheel has four positions: an open position for collecting spectra without a filter in the beam path, and three positions in which you can place a filter that you provide. See your spectrometer documentation to locate instructions for installing filters.

To specify the position to use for wheel A (the one closer to the source), select a setting from the drop-down list box at the right end of the Filter Wheel A row. To specify the wheel B position to use, select a setting from the drop-down list box at the right end of the Filter Wheel B row.

The available settings depend on the descriptions entered using the Filter Wheel table on the Configure tab. See “Entering descriptions of the filters in the filter wheel” for more information.

### Controlling the polarizer

Polarizer angle	90
-----------------	----

Use the Polarizer Angle parameter, if available on the Bench tab, to control the optional polarizer. The polarizer lets you automatically control the vibrational orientation of the infrared beam within a range of rotation from 0 to 180 degrees in increments of 1 degree. See your spectrometer documentation for more information.

To change the setting, double-click the table cell to the right of Polarizer Angle. Then type a value or click the up and down arrow buttons to the right of the value.

## Quality checks

The Quality tab contains parameters for specifying the spectral quality characteristics that you want checked when you collect spectra. OMNIC offers the four categories of spectral quality checks described below.

### Spectrum

The spectrum checks appear when you select the Spectrum (or All) option. These checks examine the quality of collected sample spectra. If you want any of these checks performed, first turn on Spectrum Checks and then turn on the checks you want performed. (Use Spectral Quality Checks must be on for these items to be available.) Set the sensitivity for each selected check by using the Sensitivity scroll bar. A higher sensitivity value makes it more likely that a problem will be detected.


### Parameter

The parameter checks appear when you select the Parameter (or All) option. These checks examine the experiment parameter settings used to collect sample spectra. If you want any of the parameter checks to be performed, first turn on Parameter Checks and then turn on the checks you want performed. (Use Spectral Quality Checks must be on for these items to be available.)


### Background

The background checks appear when you select the Background (or All) option. These checks examine the quality of collected background spectra. If you want any of the background checks to be performed, first turn on Background Checks and then turn on the checks you want performed. (Use Spectral Quality Checks must be on for these items to be available.) Set the sensitivity for each selected check that requires it by using the Sensitivity scroll bar. A higher sensitivity value makes it more likely that a problem will be detected.

**Note** If you are using a Smart Accessory experiment to collect data with a Smart Accessory, you can use Display Spectral Quality Reference in the Collect menu to display the background spectrum used to check collected backgrounds. To assign a new spectrum for this purpose, use Set New Spectral Quality Reference in the Collect menu. See “Displaying the spectral quality reference spectrum” and “Assigning a new spectral quality reference spectrum” for details. ▲

 Interferogram

The interferogram checks appear when you select the Interferogram (or All) option. These checks examine the quality of collected interferograms. If you want any of the interferogram checks to be performed, first turn on Interferogram Checks and then turn on the checks you want performed. (Use Spectral Quality Checks must be on for these items to be available.) To display a category of checks or all the checks on the Quality tab, select the appropriate option to the right of Select View.

 Use spectral quality checks

If you want any of the spectral quality checks to be performed when you collect spectra using the current experiment, turn on Use Spectral Quality Checks near the top of the dialog box. This makes the various checks available for you to select. If you don't want any checks to be performed, turn off the check box.

When OMNIC performs a check and detects a problem, the Collect Status indicator is displayed in yellow. 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 collection and other information about the collection. You can also access this information through the System Status indicator near the top of the OMNIC window. See “Viewing information about data collection problems” for more information.

For more information about the quality checks, find “quality checks” in the OMNIC Help system Index and go to the “Quality checks” topic.

**What sensitivity setting should I use?**

When you specify that a spectral quality check be used, in most cases you need to set the check's sensitivity within a range of 0 to 100. This determines how readily the check finds the problem being looked for. For example, if you turn on the H<sub>2</sub>O Levels check in the spectrum checks and then set the sensitivity to a low value, water absorptions will be found only if they are large; if you use a high value, these absorptions will be found even if they are small.

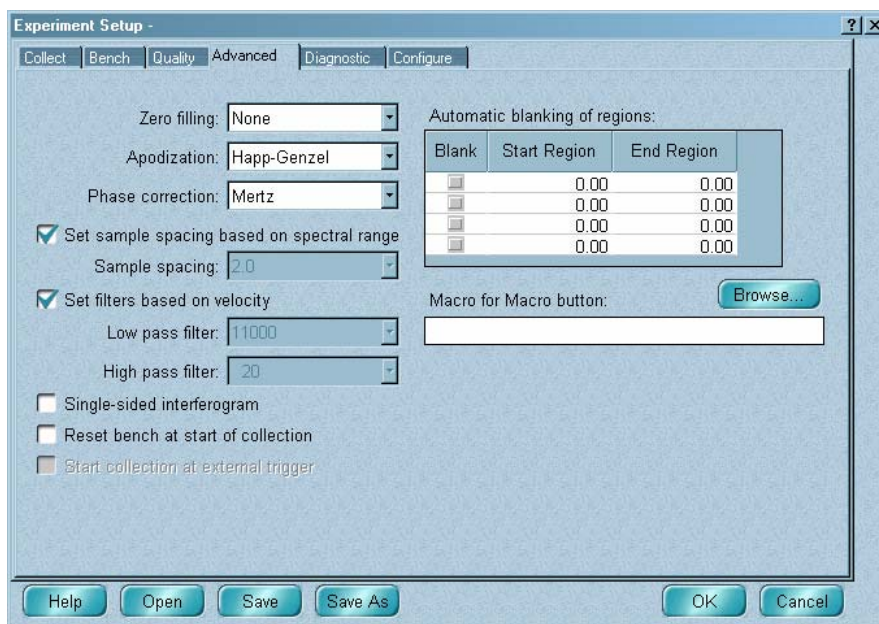


You can determine an appropriate setting for a check by first setting the sensitivity to 100 and collecting a spectrum of a typical sample under typical conditions. After the data collection, click the Collect Status indicator above the view finder or the View Collect Status button in the Confirmation message if it appears. A window shows information about the collection, including a measured value for the check. Since this value resulted from measuring a typical sample under typical conditions, you can set the sensitivity for the check slightly below this value and expect your typical data collections to pass the check in the future.

After you set the sensitivity, you can test the check to see if spectra pass or fail as expected. To do this, first collect another typical spectrum under typical conditions to see if the spectrum passes the check. Then collect a spectrum under conditions that should cause the check to fail. For example, if you set the sensitivity of the H<sub>2</sub>O Levels check based on the above procedure, you could breathe into the sample compartment and collect a sample spectrum. The spectrum should fail the check.

## Advanced parameters

The Advanced tab contains the parameters shown and described in the following illustration and table.



To specify or do this...	Use this feature...
The number of levels of zero filling.	Zero Filling
The apodization type.	Apodization
The type of phase correction to use.	Phase Correction
The sample spacing (the number of zero crossings of the reference laser).	Sample Spacing or Set Sample Spacing Based On Spectral Range
The cutoff frequency of the low pass filter.	Low Pass Filter or Set Filters Based On Velocity
The cutoff frequency of the high pass filter.	High Pass Filter or Set Filters Based On Velocity
Collect single-sided interferograms.	Single-Sided Interferograms
Reset the spectrometer interferometer at the start of data collection.	Reset Bench At Start Of Collection
Initiate data collection with an external trigger (requires special hardware).	Start Collection At External Trigger
A macro to be started with the Macro button on a Nicolet 380, Nicolet 4700, Nicolet 5700, Nicolet 6700 or Nicolet 8700 spectrometer.	Macro For Macro Button
Specify spectral regions to blank during data collection.	Automatic Blanking Of Spectral Regions

### Specifying the number of levels of zero filling

Zero filling:

Zero Filling on the Advanced tab determines the number of levels of zero filling used when the data are Fourier transformed. Zero filling improves the line shape of a spectrum by adding data points between collected data points. Sharp features become smoother and more like typical peaks when zero filling is used.

Because data points are added, the transform takes longer. Zero filling does not increase the “true” resolution of the data, however, since that is determined by the number of data points collected.

The available settings of Zero Filling are described in the following table.

Setting	Description
None	No zero filling is done.
1 Level	One data point is added between each data point.
2 Levels	This setting adds three points between each data point to better define band shapes.

Set Zero Filling to None for normal work.

Collect your sample and background spectra using the same number of levels of zero filling.

If band shapes are cut off, set Zero Filling to 1 Level or 2 Levels instead of None.

### Selecting the apodization type

Apodization:

The Apodization parameter on the Advanced tab determines the type of apodization that is used before the interferogram is Fourier transformed. Apodization removes peak side lobes that can occur because the interferogram is not an infinite set of data. The apodization types described in the following table are available. Collect your sample and background spectra using the same apodization type.

Setting	Description
Happ-Genzel	<i>This is the best choice for most applications.</i> It suppresses side lobes more effectively than the triangular type and with less reduction in resolution than that type. (It results in more reduction in resolution than the boxcar type.) Use this type if you are measuring condensed-phase samples.
Triangular	Mathematically weights interferogram data to reduce ringing effects (side lobes), resulting in lower resolution than that obtained with the boxcar and Happ-Genzel types. Some ringing will usually be present with this type. This setting is normally used only to reproduce the results of other experiments that used it.

Setting	Description
2 Levels	This setting adds three points between each data point to better define band shapes.
Boxcar	The interferogram is unweighted; that is, the data are simply truncated at the beginning and end. Use this type when you are measuring a gas sample, want maximum resolution and are not concerned about ringing effects (side lobes). The greatest amount of ringing will be present with this type.
N-B* Weak	This setting has a less pronounced smoothing effect on data than do the N-B medium and N-B strong types and degrades the resolution more than those types. This setting is generally not recommended and is normally used only to reproduce the results of other experiments that used it.
N-B* Medium	Has a smoothing effect on data which is between that of N-B weak and N-B strong. It suppresses side lobes as much as possible given that it only moderately degrades the resolution. The side lobe suppression is more significant than for N-B weak apodization. This setting is suitable for most normal samples; it gives results virtually identical to those obtained with Happ-Genzel.
N-B* Strong	This setting has a greater smoothing effect on data than do the N-B weak and N-B medium types and does not degrade the resolution of the spectrum. The side-lobe suppression is more significant than for N-B medium apodization. Side lobes appear on both sides of peaks and are more pronounced for sharper peaks. Use this setting only when the best possible resolution is required.

\* "N-B" stands for Norton-Beer.

### Specifying the phase correction

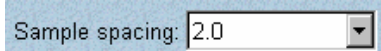
Phase correction:

Phase Correction on the Advanced tab determines the phase correction for the Fourier transformation. The following table describes the available settings.

For more information on the Mertz and Power Spectrum corrections, read *Transformations in Optics* by L. Mertz, published by John Wiley and Sons, New York, 1965.

Setting	Description
None	Uses the Mertz algorithm to calculate the phase-corrected spectrum. This is the normal setting.
Power Spectrum	Always produces a spectrum that is positive. In this correction the power equals the square root of the sum of the squares of the real and imaginary parts of the Fourier transform.
de Haseth	<p>Phase corrects vibrational circular dichroism (VCD) spectra. These spectra can have both negative and positive peaks, so the correction is designed to accommodate negative spectral features.</p> <p>This setting is available only if you have the optional SST software.</p> <p>For more information, see the article titled “Phase Correction of Vibrational Circular Dichroic Features” by Colleen A. McCoy and James A. de Haseth in the journal <i>Applied Spectroscopy</i>, Volume 42, Number 2, 1988.</p>

### Specifying the sample spacing



Sample Spacing on the Advanced tab determines the number of zero crossings of the reference laser and the allowed spectral range.

Sample Spacing is normally set to 2 (for mid-IR). If you want the spectral range to extend beyond 7899 wavenumbers, set Sample Spacing to 1 (for near-IR). If you want to reduce the processing time for a series experiment, set Sample Spacing to 4.

**Note** If you use a setting of 4, be sure to use an optical filter to filter out frequencies above 3950 wavenumbers. This prevents higher frequency peaks from being “folded over” into the actual collected range. ▲

The Sample Spacing setting affects the total number of data points collected over a given spectral range. For example, a setting of 1 doubles the number of data points as compared with a setting of 2. Similarly, a setting of 4 results in half as many data points as a setting of 2.

Set sample spacing based on spectral range

If you want the sample spacing to be set automatically based on the spectral range, turn on Set Sample Spacing Based On Spectral Range. The Sample Spacing parameter is unavailable when the check box is on.

### Specifying the cutoff frequency of the low pass filter

Low pass filter:

Low Pass Filter on the Advanced tab determines the frequency above which spectral anomalies are removed from collected data.

Setting the cutoff frequencies of filters is important when you switch to a different spectral range (near-, mid- or far-IR) or when you are working with a specific spectral region and want to maximize performance with the use of optical filters.

Use low pass filters to eliminate any high frequency noise that occurs above the optical bandwidth of the measurement. This noise is due to "folding" and occurs because the detector sampling interval is a discrete value. For a typical mid-IR scan on many system models, the interferogram is sampled at every laser crossing (a sample spacing of 1). This sets the folding noise point at the HeNe laser frequency, or approximately 15,798 wavenumbers. To prevent folding noise (noise introduced by folding of frequencies into the bandwidth of interest), a low pass filter is needed to limit the bandwidth of the detector to values below the frequency equivalent to 15798 wavenumbers. The actual frequency in hertz (Hz) that you should set the low pass filter to is a function of both the high-end wavenumber of the light and the velocity of the moving mirror. You can calculate this value by using the Fourier equation

$$\text{frequency} = 2 * \text{mirror velocity} * \text{wavenumber}$$

where mirror velocity is in cm/s and wavenumber (1/cm) represents the free spectral range.

As an example, for a standard DTGS detector operating at a mirror velocity of 0.633 cm/s and an optical cutoff at 7900 wavenumbers, the electronic filter should be set to 5 kHz (see the equation below).

$$10 \text{ kHz} = 2 * (0.633 \text{ cm/s}) * 7900/\text{cm}$$

**Note** The available settings depend on your application. The 10 kHz setting used in this example may not be available. ▲

For near-IR measurements, OMNIC automatically sets the sample spacing to every laser crossing. Thus, the free spectral range is opened up to 15,800 wavenumbers, and the low pass filter can also be opened up to a higher value (10,000 Hz in the case of our example). For visible spectroscopy, a sample spacing of one-half the HeNe frequency is also available.

Finally, there are some research applications where higher sample spacings are desirable. In such cases, pay close attention to the effects of folding on the infrared spectrum. For these sample spacing values, you must use both optical and electronic filtering to prevent folding of spectral features and noise into the desired spectrum. For more information refer to *Fourier Transform Infrared Spectrometry*, New York, John Wiley and Sons, 1986, by Peter R. Griffiths and James A. de Haseth.

Set filters based on velocity

If you want the cutoff to be set automatically based on the optical velocity, select Set Filters Based On Velocity. The Low Pass Filter parameter is unavailable when the check box is on.

**Note** If you use the SST software to perform an AM step scan, PM step scan, TRS or SMM experiment, the settings of Low Pass Filter, High Pass Filter and Set Filters Based On Velocity are ignored. ▲

### Specifying the cutoff frequency of the high pass filter

High pass filter:

High Pass Filter on the Advanced tab determines the frequency below which the effects of low-frequency noise are removed from collected data. Sources of this noise include room vibrations, fans, etc. This noise is normally a concern only when you are using a very low optical velocity, such as for a slow-scan photoacoustic measurement, or when you are collecting far-IR spectra.

You should normally set this parameter to a value equal to 1 divided by the frequency of the noise.

**Note** If you want the cutoff to be set automatically based on the optical velocity, turn on Set Filters Based On Velocity. The High Pass Filter parameter is unavailable when the check box is on. ▲

**Note** If you use the SST software to perform an AM step scan, PM step scan, TRS or SMM experiment, the settings of Low Pass Filter, High Pass Filter and Set Filters Based On Velocity are ignored. ▲

### Collecting single-sided interferograms

Single-sided interferogram

Turn on Single-Sided Interferogram on the Advanced tab if you want to collect single-sided, rather than double-sided, interferograms. This speeds up data collection and is useful when you are performing GC/IR, kinetics or other series experiments in which a large number of scans are collected during a given amount of time.

**Note** The signal-to-noise ratio will be lower when you collect data with this option turned on. ▲

### Resetting the spectrometer at the start of data collection

Reset bench at start of collection

If you find that the interferogram peak in the live display tends to drift from its normal location, turn on Reset Bench At Start Of Collection on the Advanced tab. This repositions the peak before data collection starts.

### Starting data collection with an external trigger

Start collection at external trigger

Turn on Start Collection At External Trigger on the Advanced tab if you want data collection to begin automatically when a signal is received from another application. Use this option only in specialized experiments—such as gas chromatography FT-IR—in which data collection is synchronized with some external event. Special hardware is required.

### Specifying a macro for the Macro button

Macro for Macro button:

Use Macro For Macro Button, if available on the Advanced tab, to specify a macro to be started with the Macro button on the spectrometer. You can type the pathname of the macro file in the text box, or click the Browse button and locate and select a file using the dialog box that appears.

### Blanking spectral regions during data collection

Automatic blanking of regions:

Blank	Start Region	End Region
<input checked="" type="checkbox"/>	3,250.00	3,185.00
<input type="checkbox"/>	2,655.00	2,500.00
<input checked="" type="checkbox"/>	1,870.00	1,765.00
<input type="checkbox"/>	1,235.00	1,140.00

Automatic Blanking Of Regions on the Advanced tab specifies spectral regions to be blanked so that they contain no data points in the collected spectrum. This is useful, for example, when totally absorbing bands would interfere with your viewing small sample peaks when the spectrum is displayed full scale.



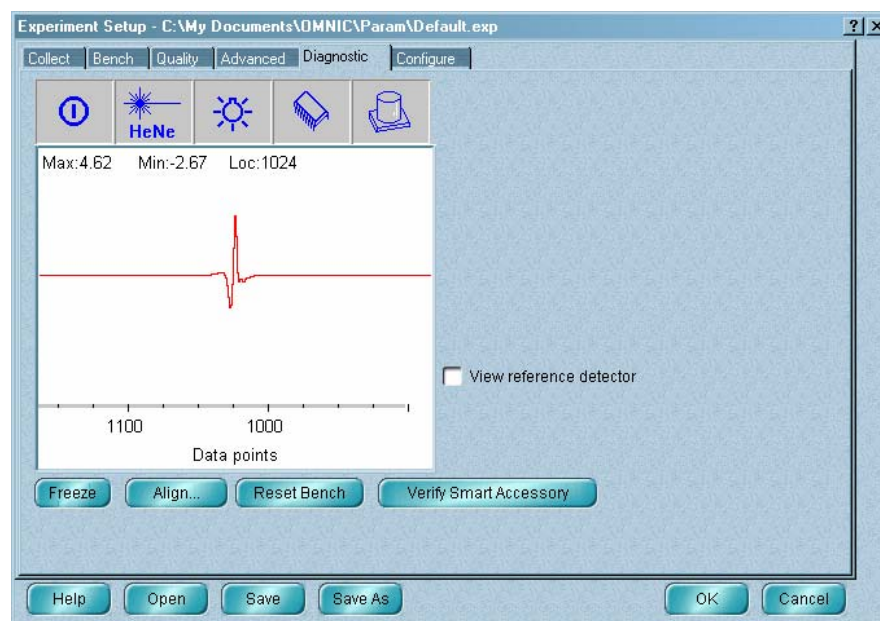
To blank a spectral region, first enter its X-axis limits in cells in the Start Region and End Region columns within a row of the table. To enter a value, click the appropriate cell and then type the desired value. Then click the check box for that row in the Blank column so that a check mark appears. Repeat this process for the other regions you want blanked, using the other rows of the table.

You can specify up to four regions and then turn their check boxes on or off as appropriate before collecting data from different samples.

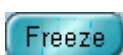
**Note** You can also blank a spectral region after data collection by using Blank in the Process menu. ▲

## Diagnostic and alignment features

When you click the Diagnostic tab, special diagnostic and alignment features appear.



At the left side of the dialog box is a live display of the detector signal. This display is similar to the live display provided on the Bench tab. See “Using the live display” for more information.



To freeze an image of the detector signal in the live display, click the Freeze button. This lets you see changes by comparing the current signal with the frozen image. If you click the button again, a frozen image of the current signal replaces the old frozen image.

Above the live display are several indicators that you can click to check the operation of spectrometer components. See “Checking spectrometer components” for more information.



Use the Check Desiccant button, if available, to check the performance of the desiccant inside the spectrometer. See “Checking the desiccant” for more information.



If your spectrometer can be aligned automatically, you can use the Align button to perform an automatic alignment of the interferometer to maximize the detector signal. See “Aligning the spectrometer” for more information.



If the interferogram peak has drifted from its normal location, you can click the Reset Bench button to reposition the peak.



If you have installed a Smart Accessory, you can display information about it by clicking the Verify Smart Accessory button.

If you have a Nicolet IR200 with a diode laser, you can use the Laser Verification button to verify the laser frequency. In OMNIC Help Topics find “laser” in the Index and go to the “Verifying the laser frequency on a Nicolet IR200” topic for details.

## Checking spectrometer components

You can check the operation of several spectrometer components by clicking the indicators located above the live display on the Diagnostic tab. The components that correspond to the indicators are named below.



Power supply



HeNe laser



Light source




Electronics




Beamsplitter and detector

**Note** The availability of the indicators depends on the spectrometer model you have. ▲

When you click one of the first four indicators, a dialog box shows information about the status of the corresponding component. (This information is not available for Mattson and IR Series spectrometers.) Each item in the first column of the dialog box is measured every second, and the measured value is displayed in the Current column.

 If this value is within the range shown in the Acceptable Range column, a check mark appears in the Status column.

 If the value is outside the acceptable range, an X appears in the Status column.

The fifth indicator lets you see the type of detector and beamsplitter currently being used.

When you are finished viewing the information, choose OK.


To troubleshoot a problem, choose Advanced Diagnostics from the Collect menu (if available) and follow the instructions that appear on the screen. For more detailed instructions, click the Help button in the Diagnostics window.


### Checking the desiccant



Use the Check Desiccant button, if available on the Diagnostic tab, to check the humidity inside the optics compartment of a sealed and desiccated spectrometer. The humidity measurement indicates how well the desiccant is performing. If the desiccant has become saturated, it no longer absorbs enough water vapor to protect the optics and should be replaced.

When you click the button, the check begins and a gauge shows its progress. When the check is complete, the results appear:

 A green check mark indicates that the desiccant is still effective. Choose OK to close the dialog box.

 A yellow circle indicates that the desiccant is no longer effective and should be replaced or renewed. Click the Explain button for instructions.

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

### Aligning the spectrometer



If your spectrometer can be aligned automatically, you can click the Align button on the Diagnostic tab to perform an automatic alignment of the interferometer to maximize the detector signal.

**Note** The spectrometer power should be on for at least 15 minutes (1 hour or longer for best results) before you perform an alignment. Aligning the system before it has warmed up and stabilized may give inconsistent results. ▲

**Notice** Set Gain to 1 before clicking the Align button. ▲

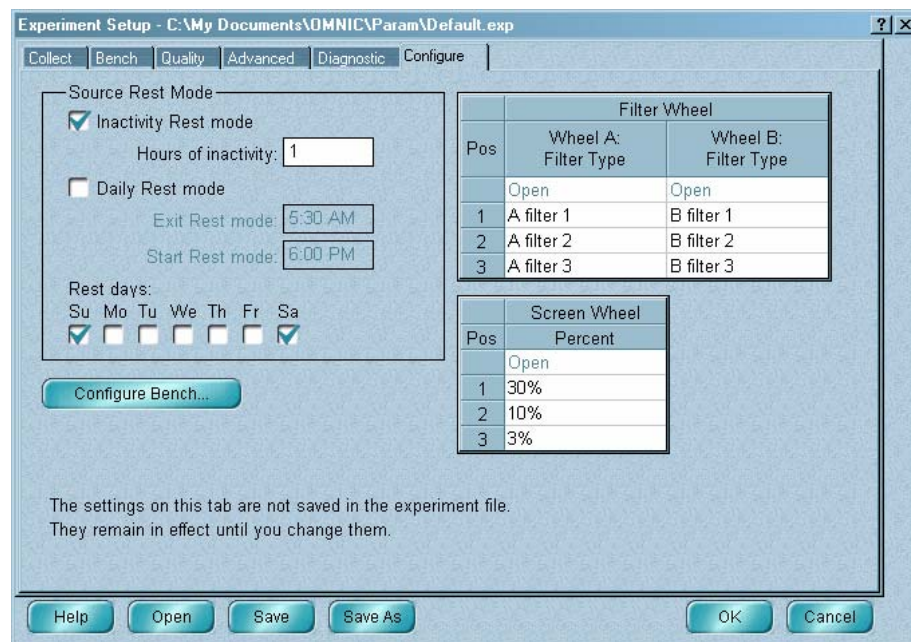
The detector signal is shown in the live display during portions of the alignment. (The signal may take a few seconds to appear, depending on your spectrometer model.) Remove any accessories or samples from the sample compartment before aligning the spectrometer.

Align the spectrometer's interferometer after installing a new beamsplitter, replacing the laser or moving the spectrometer. It is also a good idea to align the interferometer if the signal intensity has dropped significantly from its usual level.

**Note** Sampling accessories and some spectrometers must be aligned manually, not by using the Align button. If your accessory or spectrometer requires manual alignment, watch the live display on the Bench tab while making the appropriate adjustments on the accessory or spectrometer. The goal of manual alignment is to increase the maximum (Max) value above the live display to its highest possible level. See the manual that came with the accessory or spectrometer for instructions. See "Using the live display" for more information about the live display. ▲

## Configuring the system hardware

The Configure tab contains some or all of the parameters shown in the following illustration and table, depending on the model spectrometer you have.



### To specify or do this...

### Use this feature...

When to place the source into Rest mode to extend the life of the source.

Source Rest Mode features

Configure the system for the sources, beamsplitters and detectors you will be using.

Configure Bench button

Enter descriptions of the filters in the optional filter wheel.

Filter Wheel

Specify the energy screens in the optional energy screen wheel.

Screen Wheel

## Extending the life of the source with Rest mode

You can use the Source Rest Mode features on the Configure tab to extend the life of the infrared source. (A white light source cannot be placed into Rest mode.) The table below describes what Rest mode does when you are not using the source.

If you resume data collection activity when the source is in Rest mode, the source automatically leaves Rest mode so that you can collect data.

Model	Effect of Rest Mode
Nicolet iS10, Nicolet 380, Nicolet 4700, Nicolet 5700, Nicolet 6700, Nicolet 8700	Lowers the source temperature.
Magna-IR, Nicolet Nexus	Turns off the source.

### Notice

If you have a Nicolet iS10, Nicolet 380, Nicolet 4700, Nicolet 5700, Nicolet 6700 or Nicolet 8700 spectrometer, we recommend setting the Source Rest Mode features so that the source leaves Rest mode at least 15 minutes before you resume data collection. ▲

There are several ways to use Rest mode. You select one or more of them, as explained below.

- *If you want the source to enter Rest mode after a specified period of inactivity, select Inactivity Rest Mode and type the desired number of hours in the Hours Of Inactivity text box.*
- If you want the source to be in Rest mode during a specified period each day, select Daily Rest Mode and type the desired starting and ending times of the period in the Start Rest Mode and Exit Rest Mode text boxes, respectively. Use the time format that is used by your system; for example, 5:30 PM and 17:30 are two ways of expressing a starting time.
- If you want the source to be in Rest mode all day on particular days of the week, select the desired days below Rest Days.

### Note

If you select any of these options except the first one, the source will not enter Rest mode if data collection activity is occurring when the scheduled start of Rest mode is reached. This ensures that a collection that is in progress will not be spoiled by a reduction in infrared energy. ▲

## Configuring the system



You can configure the system for the hardware you are using or perform other tasks described below by clicking the Configure Bench button on the Configure tab. You must configure the system after you do any of the following:

- Install a 32-bit version of OMNIC (5.0 or greater) on a system that has been using a 16-bit version of OMNIC (earlier than 5.0).
- Install OMNIC on a spectrometer system for the first time.
- Use OMNIC with a Mattson or IR Series spectrometer for the first time.
- Install any of the following:

A new source.

A new beamsplitter (except in a Nicolet 4700; Nicolet 5700; Nicolet 6700; Nicolet 8700; Nicolet Nexus; or Magna-IR with automatically recognized interchangeable beamsplitters).

A new detector (except for Thermo Scientific detectors in a Nicolet iS10, Nicolet 380, Nicolet 4700, Nicolet 5700, Nicolet 6700, Nicolet 8700, Nicolet Nexus, Nicolet Avatar, Magna-IR or Nicolet Protégé).

A sample compartment validation wheel (Nicolet Avatar and Nicolet IR300).

Special Raman hardware in the spectrometer.

- Change the communication link between the computer and the spectrometer (except for Nicolet iS10; Nicolet 380; Nicolet 4700; Nicolet 5700; Nicolet 6700; Nicolet 8700; Nicolet Nexus; and Magna-IR upgraded for Plug and Play operation).

If you do not configure the system, you will not be able to collect data using the spectrometer.

You can do the following things when you configure the system:

- Configure and test the spectrometer-computer communication link.
- Configure your spectroscopy software for the hardware you are using.

Follow these steps to configure the system:

**1. Click the Configure Bench button on the Configure tab.**

The Bench Configuration dialog box appears. The buttons and other features that appear in this dialog box vary depending on which spectrometer is installed in the system.

**2. If the dialog box contains a Bench drop-down list box, select the model number of your spectrometer.**

Check the front of the spectrometer if you are unsure of the model number.

**3. You can configure an item by clicking the button labeled with the name of that item.**

A dialog box will appear with the features needed to configure the item.

For complete instructions for configuring your system, find “configuring” in the OMNIC Help system Index and go to the “How to configure the system” topic.

**Entering descriptions of the filters in the filter wheel**

Filter Wheel		
Pos	Wheel A: Filter Type	Wheel B: Filter Type
	Open	Open
1	A filter 1	B filter 1
2	A filter 2	B filter 2
3	A filter 3	B filter 3

Use the Filter Wheel table, if available on the Configure tab, to enter descriptions of the filters you have installed in the two wheels of the optional filter wheel accessory. See your spectrometer documentation to locate instructions for installing filters.

The Pos (for “Position”) column of the table indicates the four positions of the wheels. The other columns show the descriptions of the filters in those positions of each wheel.



The “Open” positions are used for collecting data without a filter in the beam path. You can enter descriptions of the filters in the other positions of the wheels by double-clicking the appropriate cell of the table and then typing. The descriptions you enter here will be available when you set the Filter Wheel A and Filter Wheel B parameters on the Bench tab to specify the combination of wheel positions to use for data collection. These descriptions will also appear in the collection and processing information for spectra collected using the filter wheel accessory. See “Controlling the filter wheel” for more information.

### Specifying the energy screens in the energy screen wheel

Screen Wheel	
Pos	Percent
	Open
1	30%
2	10%
3	3%

Use the Screen Wheel table, if available on the Configure tab, to enter the percentage of infrared energy transmitted by the screen in each position on the optional energy screen wheel.

The Pos (for “Position”) column of the table indicates the four numbered positions of the wheel. The other column shows the descriptions of the screens in those positions.

The “Open” position is used for collecting data without a screen in the beam path. The default descriptions of the other screens indicate the nominal percentage of energy transmitted. You can enter your own descriptions of the screens by double-clicking the appropriate cell of the table and then typing. The descriptions you enter here will be available when you set the Screen Wheel parameter on the Bench tab to specify the wheel position to use for data collection. See “Controlling the energy screen wheel” for more information.

#### — *How to* ➔

Use Experiment Setup

#### 1. Choose Experiment Setup from the Collect menu.

The Experiment Setup dialog box appears.

#### 2. Click the name of the tab that contains the features you want to use, or click the Open button to open an experiment file.

If you want to align or reset the spectrometer or check the operation of spectrometer components, click the Diagnostic tab.

**Note** The spectrometer power should be on for at least 15 minutes (1 hour or longer for best results) before you perform an alignment. ▲

If you click the Open button, the Open Experiment dialog box lists files of the Experiment Files (\*.EXP) file type. Type the name of the experiment file you want to open or select a file from the list by clicking its filename. You can change directories or drives to locate the file. The example experiment files provided with OMNIC are in the C:\My Documents\OMNIC\Param directory (or other location where you installed OMNIC).

**Note for DS systems** If Prevent Changing Directories When Opening Files is selected in the system policies, you cannot change directories or drives to locate a file to select. ▲

**Note** You can open a parameter file from an early version of OMNIC (3.0 or earlier) by first selecting the Parameter Files file type (\*.PRM) in the dialog box. After you open the file, its name will appear in the title bar with the extension .EXP and will be saved with that extension if you save the file. This prevents overwriting the parameter file. ▲

**Note** The experiments shown in the Experiment drop-down list box (if available) are those in the current experiment directory that have been opened by using Experiment Setup or by installing a Smart Accessory. If the current experiment directory is OMNIC\Param, the Default experiment provided with OMNIC is also shown. ▲

Select the parameter groups you want included when the experiment is opened. To select a group, turn on its check box in the Groups box. The table below shows what each group contains.

Group	Description
Collect	Parameters on the Collect and Quality tabs.
Bench	Parameters on the Bench tab.
Search	Parameters in the Library Setup dialog box and QCheck Setup dialog box.
Series	Parameters on the optional Series tab.
Map	Parameters on the optional Mapping tab.

If you don't include a group, those parameters will not be changed from their current settings in OMNIC.

When you have finished selecting the experiment file and parameter groups, choose OK. The experiment file is opened and the parameter settings are changed as specified. If you selected a group that was not saved in the experiment file, a message informs you.

### 3. Change the parameter settings as desired, or use the Diagnostic tab features.

**Notice** Set Gain to 1 on the Bench tab before clicking the Align button on the Diagnostics tab to align the spectrometer. ▲

### 4. When you are finished setting the parameters, you can save your settings in an experiment file.

**Note for DS systems** You may be prompted to digitally sign a file during this step. Follow the instructions that appear on the screen. Also, if Prevent Overwriting Of Files is selected in the system policies (in Security Administration), the Save Experiment As dialog box always appears when you click the Save button (see below). ▲

- To save the settings in the current experiment file (identified by the filename shown in the title bar of the Experiment Setup dialog box), click the Save button.
- To save the settings in a file with a new name, click the Save As button. The Save Experiment As dialog box appears. Type a name for your experiment file. If you don't want to use the path shown, select a directory or drive from the list.

**Note** Before you use the Save As button, we recommend that you change the title and possibly the description of the experiment on the Collect tab so that the new experiment can be distinguished from the original. ▲

**Note for DS systems** If Prevent Changing Directories When Opening Files is selected in the system policies, you cannot change the path. ▲

If you want the experiment you are saving to be the default experiment, turn on the Set As Default Experiment check box. The next time you log into OMNIC, that experiment will be selected automatically.

**Note** You can specify a default directory for this operation in the File options. The directory you specify also determines which experiments are listed in the Experiment drop-down list box. See “Specifying directories” in the “Edit” chapter for more information. ▲

If you want the experiment saved so that it can be opened later but not changed and saved with the changes, turn on the Read Only check box.

Select the parameter groups you want to include by turning on the appropriate check boxes in the Groups box. See step 2 for information on the parameters included in each group. When you are finished, choose OK.

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

**Note** If you want to delete an experiment file, use Delete Files in the File menu. See “Deleting files” in the “File” chapter for details. ▲

## Matching the parameter settings of a spectrum

Match Spectrum Settings in the Collect menu lets you quickly set the parameters in the Experiment Setup dialog box to the values that were used to collect the selected spectrum. This is useful when you want to collect a spectrum using the same conditions as those that were in effect when an existing spectrum was collected.

**Note** The Detector and Beamsplitter parameter settings are not changed. ▲

See “Using Experiment Setup” for complete information on the affected parameters.

### ➤ *How to* ➡

Match the parameter settings of a spectrum

1. **Select the spectrum whose settings you want to match.**
2. **Choose Match Spectrum Settings from the Collect menu.**

The affected parameters in the Experiment Setup dialog box are changed to match the selected spectrum.

## Displaying the optical layout

If you have a Nicolet Nexus spectrometer, you can use Show Optical Layout in the Collect menu to display a simulated three-dimensional image of the optical components inside the spectrometer and any installed major accessories. You can see the path of the infrared beam and select detectors and sources by clicking them. Click the How To button above for complete instructions.

### — How to ➡

Display and use the optical layout

#### 1. Choose Show Optical Layout from the Collect menu.

A 3-D image of the system components appears. A thick red line indicates the current path of the infrared beam through the system.

#### 2. Select a view of the components from the Viewpoint drop-down list box, or click the left or right arrow buttons to change the view in steps.

If you select All, a top view of all the system components appears.

The positive settings move your viewpoint toward the right, with 90 displaying the right side of the system, from a somewhat elevated viewpoint. Similarly, the negative settings move your viewpoint toward the left, with -90 displaying the left side.

#### 3. To see what type of detector or source is installed in a location, move the mouse cursor over the image of the component.

Changing the viewpoint first may make it easier to see the component.

#### 4. To select a detector or source, click it.

One or more mirrors move to change the beam path, and the Detector or Source parameter in the Experiment Setup dialog box is reset to your selection.

If you have a Continuum™ or Nic-Plan™ microscope, you can select reflection mode or transmission mode by clicking the upper or lower objective, respectively. Mirrors in the microscope move to change the beam path, and the Sample Compartment parameter in the Experiment Setup dialog box is reset to your selection.

#### 5. When you are finished viewing the optical layout, click the Close button in the upper-right corner of the window.

## Collecting a sample spectrum

After you have selected an experiment, use Collect Sample in the Collect menu to collect the spectrum of a sample. This command works differently depending on which final format and background options are currently selected and how the Collect options are set in the Options dialog box (see “Collect parameters” in this chapter and “Collect options” in the “Edit” chapter for details). You may be prompted during collection to take the appropriate action; for example, to prepare to collect a background spectrum or to enter a title for the collected spectrum. Follow the instructions that appear on the screen.

During collection a live display of the data appears in the Collect Sample window. (For some spectrometer models, a message describing the progress of the collection appears instead.)

## Viewing the progress of the collection



The progress of the collection is indicated visually by the gauge at the left side of the window just below the pane. As data are collected, the gauge is gradually filled with black from left to right. For some spectrometers the number of scans collected so far and the total number of scans for the collection are displayed to the right of the gauge.

## Viewing information about data collection problems

During and after collection the Collect Status indicator above the view finder shows the status of the collection. To view information about the collection, including any problems that have occurred, click the indicator after pausing the collection (explained below) or click the View Collect Status button in the Confirmation message if it appears following the collection.

**Note** On some Mattson and IR Series spectrometers, the quality checks are not performed until data collection is finished. ▲



If the indicator shows a green check mark, the spectrum has passed all of the selected spectral quality checks. If the indicator is a green check mark after the collection is finished, you can add the spectrum to a spectral window (if it is not automatically added).



If the indicator is a yellow shield containing an exclamation mark, 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 shows a red X, there is a problem with the quality of the spectrum. After correcting the problem, collect the spectrum again.

When you click the View Collect Status button at the end of data collection or click the Collect Status indicator, the Collect Status dialog box shows a summary of data collection problems encountered during the collection and other information about the collection. A brief description of each problem is given, along with the measured values and the allowed values specified for the quality check that found the problem. The Explain button lets you display information on solving the problem.

**Note** To specify the quality checks you want performed during data collection, use the Quality tab in the Experiment Setup dialog box. See “Quality checks” for details. ▲

You can copy the displayed information to the Windows Clipboard by choosing Copy. You can then paste the information into a word processing program.

To print the displayed information, choose Print.

To close the Collect Status dialog box, choose Close.

## Viewing the resolution of the data

The resolution of the data is displayed to the right of the total number of scans.

## Viewing the age of the background

The time elapsed since the current background spectrum was collected is shown in the box that says “Bkg Age.”

## Displaying a different spectral region

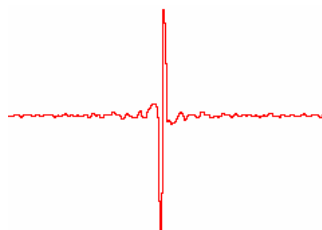
Use the view finder if you want to display a different region. See “View finder” in the “About the Display” chapter if you need help.

## Displaying the peak intensity or the noise in a spectral region

The peak intensity of the last scan is displayed below the pane as the “Peak Value.” To see the noise level in a region of the spectrum being collected, use the region tool to select the desired region. The noise value will be displayed below the pane instead of the peak value.

## What happens during collection?

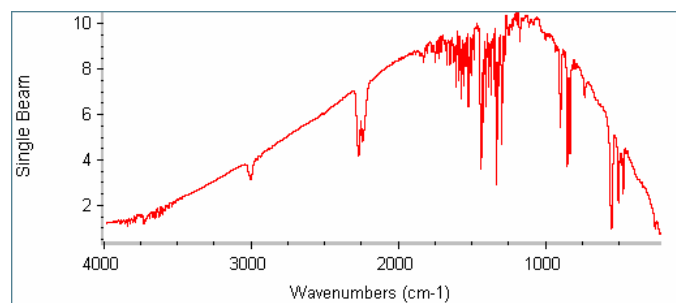
The interferogram (see the example below) is the signal measured by a Fourier transform infrared (FT-IR) spectrometer.



The interferogram shows the signal intensity in volts (Y-axis) versus the displacement of the moving mirror measured in data points (X-axis). If you collect more than one scan, the system averages all of the data to improve the signal-to-noise ratio of the measurement. For more information on signal averaging, see “Specifying the number of scans.”



The interferogram is Fourier transformed into a single-beam spectrum (see the following example).

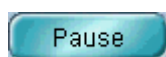


### Single-beam sample spectrum

The sample single-beam spectrum shows how the energy of the source is distributed over the displayed frequency range. It includes the characteristics of the detector, beamsplitter and atmospheric conditions along with those of the sample. To isolate the features due to the sample, a second single-beam spectrum, called a background, is collected under the same conditions but without the sample.

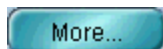
Finally, the single-beam spectrum of the sample is ratioed against the single-beam spectrum of the background. This step eliminates the background characteristics of the spectrometer so that the peaks in the final spectrum are due solely to the sample.

## Pausing and continuing data collection



The Pause button in the Collect Sample window lets you pause data collection before all the scans have been collected. After you pause the collection, you can add the spectrum to a spectral window using the window selection box. When you choose Pause, the button changes to the Continue button. To continue data collection where it left off, choose Continue. The button will change back to the Pause button.

## Collecting additional scans



If you choose More Scans when asked whether to add the spectrum to a spectral window, you can then click the More button near the Collect Status indicator to collect additional scans. They will be averaged with the data collected so far, thereby improving the signal-to-noise ratio. When you choose More, a dialog box lets you enter the number of additional scans you want to collect. After you enter a number and choose OK, data collection resumes and the More button becomes the Pause button. When all the additional scans have been collected, the button changes back to the More button.

### — How to ➔

Collect a sample spectrum

1. Use **Experiment Setup** in the **Collect** menu to check the settings of the experiment parameters.

If the parameters are not set the way you want them, change the settings now or open an appropriate experiment file. When you are finished setting the parameters, choose OK.

#### Note

You can also select an experiment from the Experiment drop-down list box near the top of the OMNIC window. ▲

#### ⚠ Warning

*Never* stare into the laser beam or at its bright reflection. ▲

2. If **Prompt To Insert Or Remove Sample** is turned off in the **Collect options** (available through **Options** in the **Edit** menu) do one of the following:

- If you will be collecting a background first, make sure the system is ready. (For example, if the application requires that the background be collected with the beam path clear, remove any sample from the path.)
- If you will not be collecting a background spectrum first, install the sample.

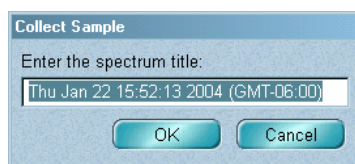
A background spectrum will be collected first if you have turned on **Collect Background Before Every Sample** in the **Experiment Setup** dialog box.

Skip this step if **Prompt To Insert Or Remove Sample** is turned on.

**3. Choose Collect Sample from the Collect menu and then follow the instructions that appear on the screen.**

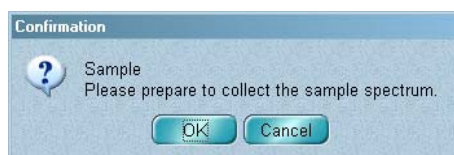
If Preview Data Collection is turned on in the Experiment Setup dialog box, preliminary data collection begins and the data are displayed in the Collect Sample window. If you are satisfied with the data, start the actual sample data collection by clicking the Start Collection button. If you don't want to collect a sample spectrum, click the Stop button to end the procedure.

- If the following message appears, type a title for the spectrum and then choose OK or accept the default title in the text box by just choosing OK.



If you choose Cancel, the data collection procedure will end.

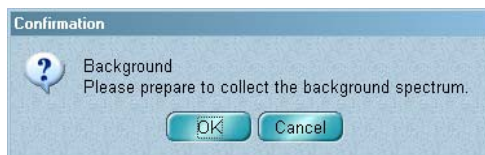
- If the following message appears, install your sample in the appropriate sample holder or accessory and then choose OK.



If you choose Cancel, the data collection procedure will end.

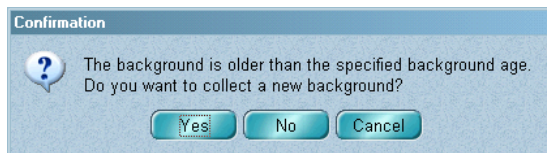
**Note** If your spectrometer is being purged, after installing the sample wait until the purge has reached equilibrium before choosing OK. The time needed to reestablish equilibrium depends on how long the sample compartment was open when the sample was inserted and when a background spectrum was last collected. Three to five minutes is usually adequate. ▲

- If the following message appears, remove any sample from the beam path (or install the background material) and then choose OK.



If you choose Cancel, the data collection procedure will end.

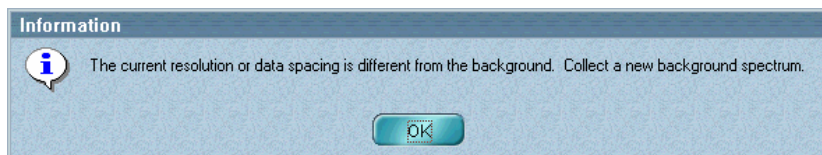
- If the following message appears, choose Yes if you want to collect a new background and then follow the instructions that appear on the screen.



If you choose No, sample data collection continues. The current background will be used to ratio the sample spectrum (if necessary to obtain the specified final format).

If you choose Cancel, sample data collection ends. You can then collect a new background using Collect Background in the Collect menu or perform other tasks. To specify a different background age, use Experiment Setup in the Collect menu.

- If the following message appears, choose OK to collect a new background and then follow the instructions that appear on the screen.



- If data collection is finished and the Collect Sample window is displayed, you can move the spectrum to a spectral window so that you can use it in operations. To do this, select the desired option from the window selection box at the top of the Collect Sample window and then choose Add.

**Note** You can select an option from the window selection box while data are being collected. You will be asked if you want the collected spectrum placed in the window you specified. ▲

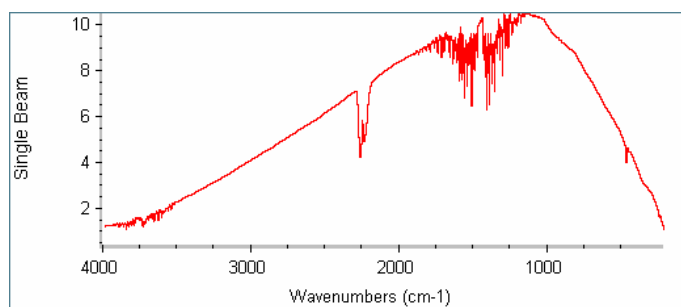
If you don't want to move the spectrum to a spectral window, close the Collect Sample window.

- If a message asks whether to add the spectrum to a spectral window, choose Yes to add the spectrum to the indicated window; choose No to end the procedure without saving the spectrum; or choose Cancel to return to the Collect Sample window. To view information about collection problems, choose View Collect Status.

**Note** To store the spectrum on the hard disk after moving it to a spectral window, use Save As in the File menu. See "Saving spectra using new filenames" in the "File" chapter for details. ▲

## Collecting a background spectrum

Use Collect Background in the Collect menu to collect a background spectrum (see the example below). A background spectrum measures the response of the spectrometer without a sample in place. During collection a live display of the data appears in the Collect Background window. (For some spectrometer models, a message describing the progress of the collection appears instead.)



**Note** Experiment Setup provides several options for determining when and how a background spectrum is collected. Depending on the Background Handling option selected, you may never need to use the Collect Background command. See "Background handling" for more information. ▲

The background spectrum you use to process your sample spectra should contain the same information about the conditions inside the spectrometer as the sample spectra. If the conditions change over time, a new background may be needed.

A background spectrum is used to eliminate signals due to the spectrometer and its environment from the sample spectrum. The background single-beam spectrum shows how the energy of the source is distributed over the displayed frequency range. It includes the characteristics of the environment of the spectrometer, including the detector, beamsplitter and atmospheric conditions.

Each sample single-beam spectrum is ratioed against the background single-beam spectrum so that the absorptions in the final spectrum are due solely to the sample. The sample spectrum is displayed using the specified final format; for example, absorbance or % transmittance.

## **When to collect a new background spectrum**

Collect a new background spectrum if...

- You have changed the hardware in your spectrometer.
- You have changed the settings of any of the following parameters in the Experiment Setup dialog box.

On the Collect tab: Resolution, Automatic Atmospheric Suppression.

On the Bench tab: Optical Velocity, Aperture, Sample Compartment, Detector, Beamsplitter, Source, Accessory, Window, Max Range Limit, Min Range Limit.

On the Advanced tab: Zero Filling, Apodization, Sample Spacing, Phase Correction, Low Pass Filter, High Pass Filter, Single-Sided Interferogram.

- There is a change in the size of the water or carbon dioxide bands in your sample spectra.
- You are about to collect a sample spectrum to use as a standard in a quantitative analysis method.

- You are about to collect a sample spectrum to use to calculate the concentrations of components in some samples.

### **A tip for demanding applications**

You can obtain the best results by collecting sample and background spectra under similar conditions. If your usual procedure for collecting sample spectra is to install the sample, allow the system to purge for three to five minutes, and then choose Collect Sample, try opening and closing the sample compartment (to let in some room air) and then waiting three to five minutes before choosing Collect Background. Since the spectra will have been collected under similar atmospheric conditions, the absorptions due to gases inside the spectrometer will be cleanly removed when the sample spectrum is ratioed against the background. ▲

### **Viewing the progress**



The progress of the collection is indicated visually by the gauge at the left side of the window just below the pane. As data are collected, the gauge is gradually filled with black from left to right. For some spectrometers the number of scans collected so far and the total number of scans for the collection are displayed to the right of the gauge.

### **Viewing the resolution**

The resolution of the data is displayed to the right of the total number of scans.

### **Viewing the age of the background**

The time elapsed since the current background spectrum was collected is shown in the box that says “Bkg Age.”

### **Displaying a different spectral region**

Use the view finder if you want to display a different region. See “View finder” in the “About the Display” chapter if you need help.

### **Displaying the peak intensity or the noise in a spectral region**

The peak intensity of the last scan is displayed below the pane as the “Peak Value.” To see the noise level in a region of the spectrum being collected, use the region tool to select the desired region. The noise value will be displayed below the pane instead of the peak value.

## Viewing information about data collection problems

During and after collection the Collect Status indicator above the view finder shows the status of the collection. To view information about the collection, including any problems that have occurred, click the indicator after pausing the collection (explained below) or click the View Collect Status button in the Confirmation message if it appears following the collection.

**Note** On some Mattson and IR Series spectrometers, the quality checks are not performed until data collection is finished. ▲



If the indicator shows a green check mark, the spectrum has passed all of the selected spectral quality checks. If the indicator is a green check mark after the collection is finished, you can add the spectrum to a spectral window (if it is not automatically added).



If the indicator is a yellow shield containing an exclamation mark, 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 shows a red X, there is a problem with the quality of the spectrum. After correcting the problem, collect the spectrum again.

When you view information about a collection problem, it is displayed in the Collect Status dialog box.

## The current background

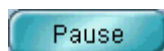
Sample spectra are ratioed against the current background spectrum. The current background is the background spectrum that was collected last (and is now in memory) or that is specified by Use Specified Background File in the Experiment Setup dialog box. This option lets you select a background from those stored on the hard disk (see “Background handling” for details). If you collect and save a new background, it will be available when you select a background handling option.

**Note** When you collect a background spectrum, it becomes the current background regardless of whether you place it into a spectral window following collection. ▲

**Note** If Use Specified Background File is currently on, you will not be able to collect a new background until you select a different background handling option. ▲

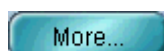


## Pausing and continuing data collection



The Pause button in the Collect Background window lets you pause data collection before all the scans have been collected. After you pause the collection, you can add the spectrum to a spectral window using the window selection box. When you choose Pause, the button changes to the Continue button. To continue data collection where it left off, choose Continue. The button will change back to the Pause button.

## Collecting additional background scans



When data collection is finished, the Pause button changes to the More button. The More button lets you collect additional scans. They will be averaged with the data collected so far, thereby improving the signal-to-noise ratio. When you choose More, a dialog box lets you enter the number of additional scans you want to collect. After you enter a number and choose OK, data collection resumes and the More button changes to the Pause button. When all the additional scans have been collected, the button changes back to the More button.

### — *How to* ➔

Collect a background spectrum

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

### ▲ **Warning**

*Never* stare into the laser beam or at its bright reflection. ▲

2. **Use Experiment Setup in the Collect menu to check the experiment parameters.**

If the parameters are not set the way you want them, change the settings now or open an appropriate experiment file. If you are using a sampling accessory, set the parameters so that the background is measured through the accessory. When you are finished setting the parameters, choose OK.

### **Note**

You can also select an experiment from the Experiment drop-down list box near the top of the OMNIC window. ▲

3. **Choose Collect Background from the Collect menu.**

The Collect Background window appears. Follow the instructions that appear on the screen.

If Preview Data Collection is turned on in the Experiment Setup dialog box, preliminary data collection begins and the data are displayed in the Collect Background window. If you are satisfied with the data, start the background data collection by clicking the Start Collection button. If you don't want to collect a background spectrum, click the Stop button to end the procedure.

- If a message asks you to prepare to collect the background, remove any sample from the beam path (or install the background material) and then choose OK. If you choose Cancel, the data collection procedure will end.
- If data collection is finished and the Collect Background window is displayed, you can move the spectrum to a spectral window so that you can use it in operations. To do this, select an option from the window selection box at the top of the Collect Background window and then choose Add.

**Note** You can select an option from the window selection box while data are being collected. You will be asked if you want the collected spectrum placed in the window you specified. ▲

**Note** If you don't want to add the spectrum to a spectral window, close the Collect Background window. The spectrum is not saved but remains the current background. ▲

- If a message asks whether to add the spectrum to a spectral window, choose Yes to add the background spectrum to the indicated window; choose No to end the procedure without saving the spectrum; or choose More Scans to return to the Collect Background window. To view information about collection problems, choose View Collect Status.

**Note** If you want this background to be available when you select a background handling option later, use Save As to save it on the hard disk after adding it to a spectral window. See "Saving a spectrum using a new filename" in the "File" chapter for more information. ▲

## Displaying the current background spectrum

Use Display Background in the Collect menu to display a copy of the current background spectrum in the active spectral window. This lets you visually check the quality of the background and look for water and carbon dioxide or other contaminants. Using a background spectrum of poor quality or one collected with another technique will often cause undesirable spectral features to appear in your sample spectra.

**Note** The current background in memory is not affected by changes you make to the displayed copy of it. ▲

**Note** Since there must be a spectral window in which to display the background spectrum, the command is not available if no spectral window exists. You can use New Window in the Window menu to create a spectral window. See “Creating a spectral window” in the “Window” chapter if you need help. ▲

### ■ *How to* ➔

Display the current background spectrum

#### 1. **Select the spectral window in which you want the background displayed.**

If only one spectral window currently exists, that is the selected window. You can use New Window in the Window menu to create a spectral window if no spectral window exists.

#### 2. **Choose Display Background from the Collect menu.**

The current background spectrum is displayed.

## Displaying the spectral quality reference spectrum

Use Display Spectral Quality Reference in the Collect menu to display a copy of the current spectral quality reference spectrum. This is the background spectrum that is associated with the current Smart Accessory experiment. The spectrum should be a “good” spectrum for the application being used. When you collect data with the experiment (using the appropriate Smart Accessory), this spectrum is used when the quality of background spectra is checked. See “Quality checks” for descriptions of the background checks.

By displaying and comparing the spectral quality reference spectrum with a background spectrum collected using the experiment, you can visually verify problems reported by the background checks.

**Note** You can designate a new spectral quality reference spectrum for an experiment by using Set New Spectral Quality Reference in the Collect menu. See “Assigning a new spectral quality reference spectrum” for details.

▲

### — *How to* ➔

Display the spectral quality reference spectrum

1. **Select the experiment whose spectral quality reference spectrum you want to display.**
2. **Choose Display Spectral Quality Reference from the Collect menu.**

The spectrum is displayed in the active spectral window, or in a new spectral window if no spectral window exists.

## Assigning a new spectral quality reference spectrum

Use Set New Spectral Quality Reference in the Collect menu to designate the selected background spectrum as the spectral quality reference spectrum for the current Smart Accessory experiment. When you collect data with the experiment (using the appropriate Smart Accessory), this background spectrum will be used when the quality of background spectra is checked. See “Quality checks” for descriptions of the background checks.

**Notice** Since the assigned spectrum will be the standard by which newly collected background spectra are judged, be sure to use a spectrum collected under normal system conditions. The accessory you use should be properly installed and aligned, any ATR crystal or sample cell you use should be in good condition, etc. ▲

If at any time the system conditions have changed, making the current spectral quality reference spectrum no longer appropriate for checking background spectra, use this command to assign a new spectrum.

**Note** You can display the current spectral quality reference spectrum by using Display Spectral Quality Reference in the Collect menu. See “Displaying the spectral quality reference spectrum” for details. ▲

**— How to ➡** Assign a new spectral quality reference spectrum

1. **Select the experiment whose spectral quality reference spectrum you want to assign.**

See “Selecting an experiment” if you need help.

2. **Select the displayed background spectrum you want to designate as the spectral quality reference spectrum.**

You can collect a background spectrum for this purpose or open one that is stored on a disk.

3. **Choose Set Spectral Quality Reference from the Collect menu.**

## Using the advanced diagnostics

Use Advanced Diagnostics in the Collect menu to troubleshoot problems with the spectrometer.

**— How to ➡** Use the advanced diagnostics

**Choose Advanced Diagnostics from the Collect menu.**

Follow the instructions that appear on the screen. For more detailed instructions, click the Help button in the Diagnostics window.



# View

Use the commands in the View menu to look at your spectral data in different ways:

To do this...	Use this command...
Undo display limit changes in a spectral window.	Undo Limit Change
Restore display limit changes reversed with Undo Limit Change.	Redo Limit Change
Set the display parameters for a spectral window.	Display Setup
Stack spectra in a spectral window.	Stack Spectra
Overlay spectra in a spectral window.	Overlay Spectra
Hide a spectrum from view.	Hide Spectra
Adjust the vertical scale of spectra so that they fit their panes.	Full Scale
Display spectra using the lowest and highest Y-axis display limits.	Common Scale
Display spectra using the Y-axis display limits of a selected spectrum.	Match Scale
Display spectra vertically offset.	Offset Scale
Specify X-axis and Y-axis display limits for spectra.	Display Limits
Display spectra full scale automatically after displaying a different spectral region.	Automatic Full Scale
Display a set of symbols for adjusting the display of spectra in spectral windows.	Roll/Zoom Window
Display the toolbar for the current configuration.	Toolbar

To do this...	Use this command...
Display the System Status Overview dialog box, which gives you access to some of the System Performance features. See “Viewing the system status” in the “Collect” chapter for details.	System Status
Access the System Status Overview dialog box with all installed features present, including options for configuring and enabling monitoring for System Performance Verification features. See “Controlling access to System Performance Verification features” in the “Collect” chapter for details.	Configure System Status

You can customize the way OMNIC displays spectra by setting options using the Options command in the Edit menu. See “Customizing OMNIC by setting options” in the “Edit” chapter for details.

## Undoing display limit changes

Undo Limit Change in the View menu lets you quickly undo changes you have just made to the display limits of a spectral window. You can undo up to six consecutive changes, one at a time, if you have not performed other operations since making the changes. The display limit changes that you can undo include those made using the following features:

- view finder
- selection tool
- Roll/Zoom window
- Redo Limit Change
- Full Scale
- Common Scale
- Match Scale
- Offset Scale
- Display Limits

### — *How to* ➔

Undo a display limit change

#### **Choose Undo Limit Change from the View menu.**

The display limits are returned to their former values. You can repeat this for up to five previous display limit changes if you did not perform other operations between the changes.



## Redoing display limit changes

Redo Limit Change in the View menu lets you quickly restore display limit changes you have just reversed with Undo Limit Change in the View menu. You can redo up to six consecutive changes, one at a time, if you have not performed other operations since undoing the changes. See “Undoing display limit changes” for more information.

### — How to —>

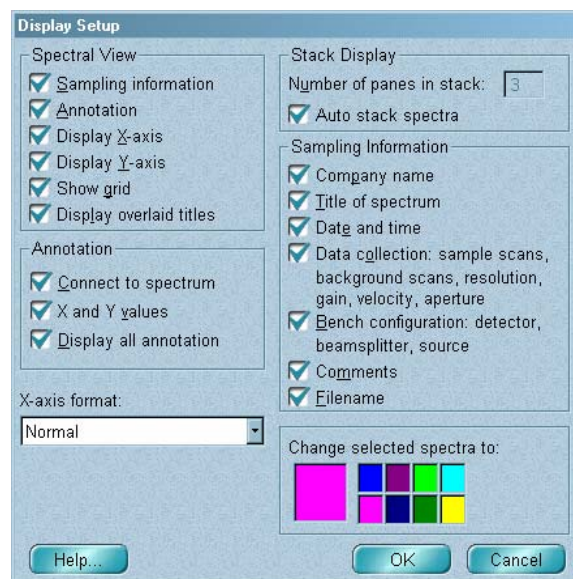
Redo a display limit change

### Choose Redo Limit Change from the View menu.

The display limits are returned to their former values. You can repeat this up five times if you did not perform other operations between undoing the limit changes.

## Setting the display parameters

Use Display Setup in the View menu to specify how spectra are to be displayed in the currently active spectral window. The display parameters are provided in the Display Setup dialog box:



**Note** If you create a new spectral window, it will use the Window options. See “Window options” in the “Edit” chapter for details. ▲

The following table shows what you can specify with each parameter.

To specify or do this...	Set this parameter...
Display information about how a spectrum was collected.	Sampling Information
Display annotations.	Annotation
Display the X-axis.	Display X-Axis
Display the Y-axis.	Display Y-Axis
Display a grid indicating X and Y values.	Show Grid
Display the titles of all overlaid spectra.	Display Overlaid Titles
Connect annotations to spectra with a line.	Connect To Spectrum
Include both the X and Y values in labels created with the annotation.	X And Y Values
Display annotations for all spectra.	Display All Annotation
The X-axis format of spectral data.	X-Axis Format
The number of panes to be used when spectra are stacked.	Number Of Panes In Stack
Adjust the number of stacked panes to match the number of spectra.	Auto Stack Spectra
The kinds of information included when sampling information is displayed.	Sampling Information
The color used to display spectra.	Change Selected Spectra To

The following sections describe the display parameters in detail. The step-by-step procedure that appears later explains how to set each parameter.

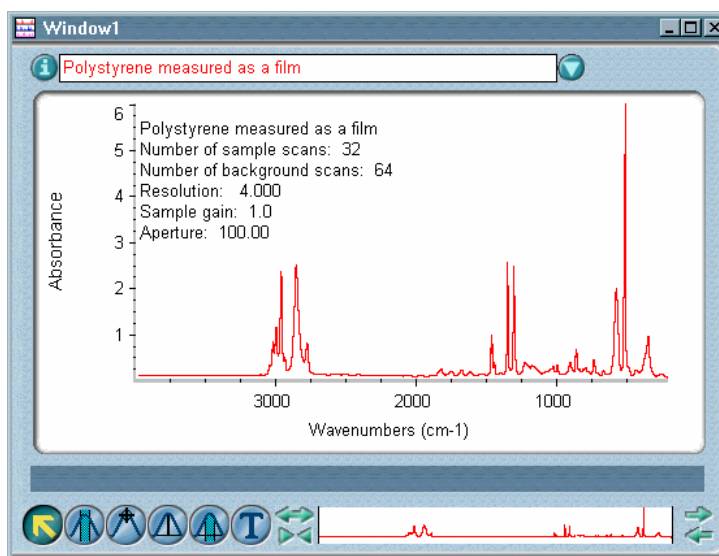
## Spectral View

This section explains the options available in the Spectral View box.

### Displaying sampling information

Sampling information

Whenever you collect a spectrum, information about how the spectrum was collected is included with the data. The Sampling Information option determines whether this information is displayed for the most recently selected spectrum that is currently displayed in the spectral window or for all the displayed spectra in the window if they are stacked. The information for a spectrum is displayed within the spectrum's pane:

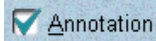


**Note** You can also view sampling information for the selected spectrum by clicking the Information button (labeled “i”) to the left of the title box or by double-clicking the spectrum’s title in the title box. The information is displayed in the Collection And Processing Information window. See “Collection and processing information” in the “About the Display” chapter for details. ▲

The Sampling Information box lists the kinds of information that can be saved with a spectrum and displayed. (Both the Sampling Information option and the desired items in the Sampling Information box must be turned on for sampling information to be displayed.) See “Specifying the sampling information to display” for details.

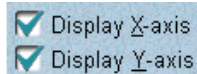
If you print a spectrum when its sampling information is displayed, the information is printed also.

### Displaying annotations



Turn on Annotation if you want to be able to add annotations to spectra with the palette tools and display existing annotations, including labels you have added using Find Peaks in the Analyze menu. To specify how to display annotations, select the desired options in the Annotation box. See “Specifying how to display annotation” later in this chapter, “Annotation tool” in the “About the Display” chapter and “Finding peaks” in the “Analyze” chapter for more information.

### Displaying the axes

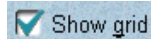


Turn on Display X-Axis and Display Y-Axis if you want the X-axis and Y-axis, including their units, displayed in the active spectral window. The axes are normally displayed.

#### Note

When you print the contents of a spectral window, you can specify whether the axes are printed by setting options in the Axes box in the Print options. See “Specifying how to print axes” in the “Edit” chapter for details. ▲

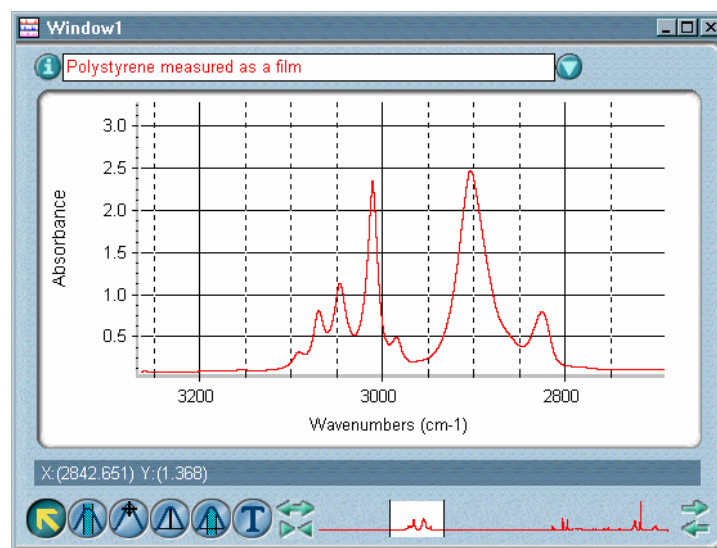
### Displaying a grid



If you want a grid displayed in each stacked pane or in the active overlaid pane of the active spectral window, turn on Show Grid. The grid is composed of vertical and horizontal lines that represent values on the X-axis and Y-axis. The major grid lines are aligned with the tick marks labeled with axis values, and the minor lines are evenly spaced between the major lines. The lines make it easier to find the X and Y values of points in the spectra and can be an aid in spectral interpretation.

Here is an example:

To remove the grid from a spectral window, turn off Show Grid.

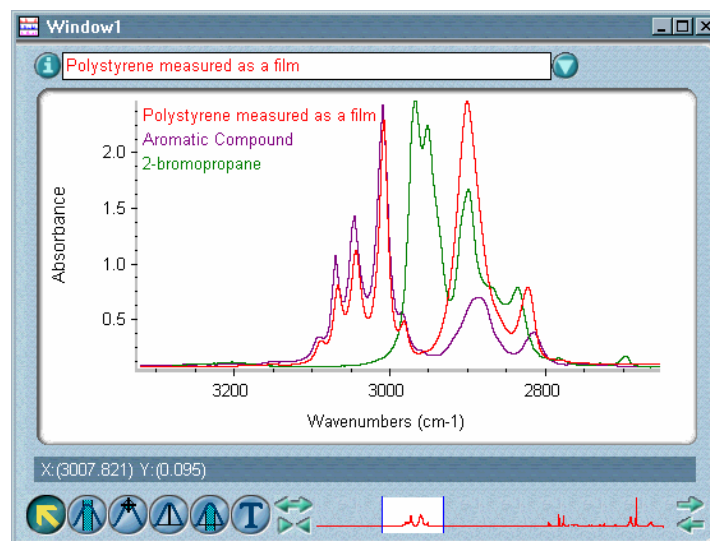


**Note** If you want a grid to be printed with spectra or included when you paste a spectrum into a log, turn on Show Grid in the Print options (available through Options in the Edit menu). See “Specifying how to print axes” in the “Edit” chapter for details. ▲

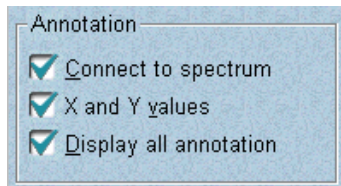
### Displaying overlaid titles

Display overlaid titles

If you want the titles of all the overlaid spectra in the active spectral window to be displayed in their panes at all times, turn on Display Overlaid Titles. The titles will appear in the upper-left corner using the same colors as the corresponding spectra and will be vertically offset to make them readable. Here is an example:

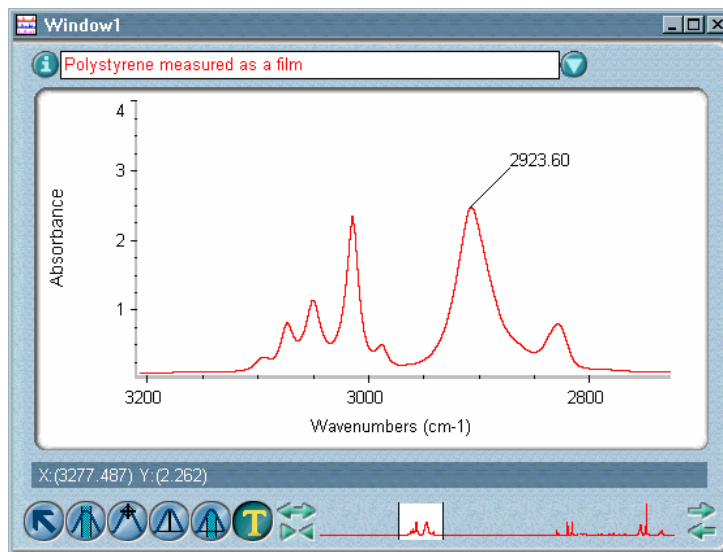


## Specifying how to display annotations



If the Annotation option in the Spectral View box is turned on, you can use the options in the Annotation box to specify how to display labels and other annotations. See “Displaying annotations” for more information on the Annotation option.

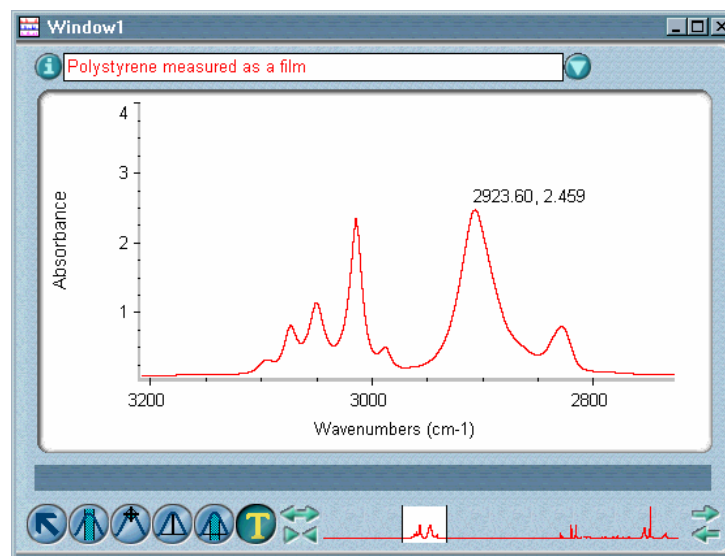
Turn on Connect To Spectrum if you want new annotations you create with the palette tools to be connected to the spectrum with a line. Here is an example:



**Note** A label created using Find Peaks in the Analyze menu will always be connected to the spectrum with a line if you move the label away from the spectrum. ▲

Turn on X And Y Values to display both the X and Y values of the point you are annotating with the annotation tool instead of just the X value. (You can still edit the annotations after you create them.)

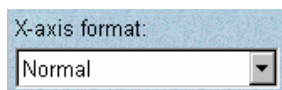
Here is an example:



Turn on Display All Annotation to display the annotations for all the displayed spectra in the active spectral window instead of just for the selected spectrum.

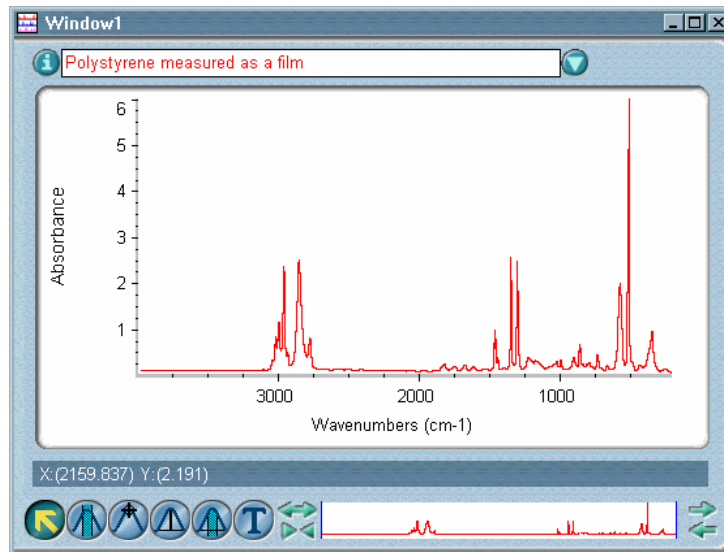
**Note** You can display annotations vertically or horizontally and specify a font for the text by using the View options (available through Options in the Edit menu). See “View options” in the “Edit” chapter for details. ▲

### Selecting an X-axis format



Use X-Axis Format to specify how to display the X-axis. The following settings are available.

**Normal** – In this format (see the following example) spectra are displayed in wavenumbers, and the X-axis uses the same scale for its entire displayed range (4000 to 400 wavenumbers, unless you have adjusted the display). This is the most commonly used X-axis format and is suitable for displaying mid- and far-IR spectra. These spectra are easier to view in this format than in the Wavelength ( $\mu\text{m}$ ) format since the peaks are displayed more spread out than in those formats.

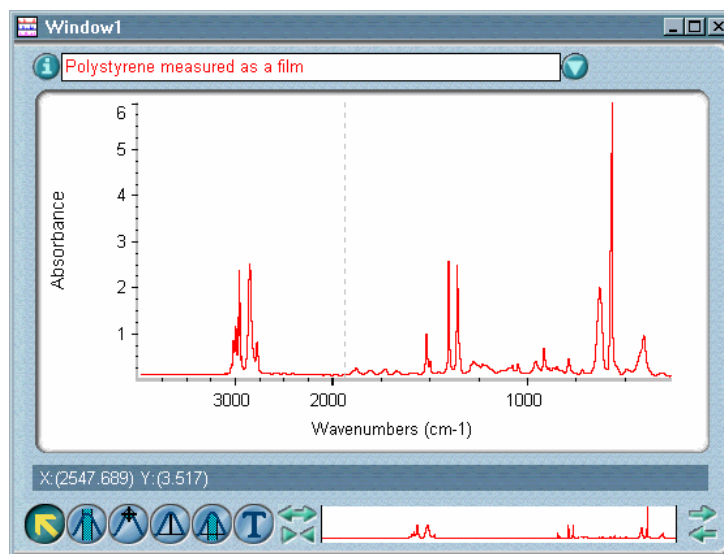


Wavenumber (the number of waves per centimeter) is the reciprocal of wavelength (the distance between corresponding points in consecutive waves):

$$\text{wavenumber} = 1/\text{wavelength}$$

**Split At 2000  $\text{cm}^{-1}$**  – In this format (see the following example) spectra are displayed in wavenumbers, and the X-axis is split into two regions with a change of scale at 2000 wavenumbers. (A vertical dashed line appears at the split.) The scale of the region below 2000 wavenumbers is expanded by a factor of 2 as compared with the scale of the region above 2000 wavenumbers.

This format was commonly used in the past to display and plot data collected using dispersive spectrometers.



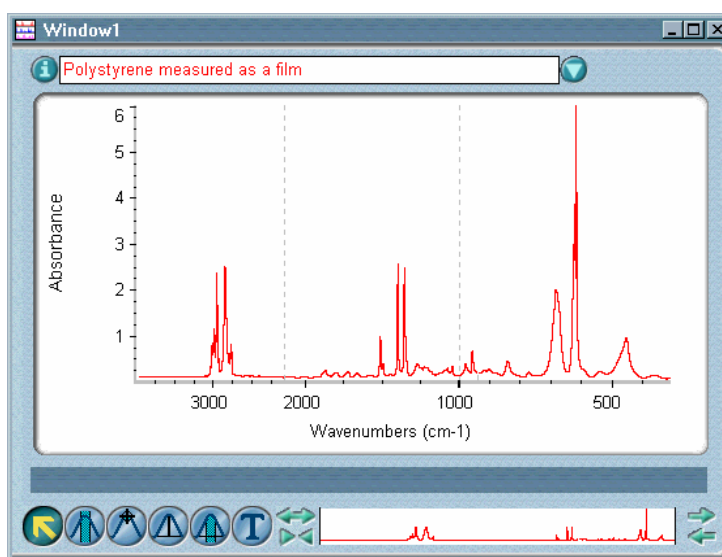


This format is useful for spectral interpretation. The region below 1,500 wavenumbers is the “fingerprint” region. Here you can find characteristic peaks that confirm your identification of the compound. Expanding this region with the Split At 2000  $\text{cm}^{-1}$  format makes it easier to view these peaks. This region is also where you can observe the spectral effects of molecular bending.

The region above 1,500 wavenumbers is called the “functional group region” and is where you can observe the effects of molecular vibrational stretching.

**Split At 2200 And 1000  $\text{cm}^{-1}$**  – In this format spectra are displayed in wavenumbers, and the X-axis is split into three regions, each with a different scale. (A vertical dashed line appears at each split.) As you move from left to right, the scale of each region is expanded by a factor of 2 as compared with the scale of the region to its left. Here is an example:

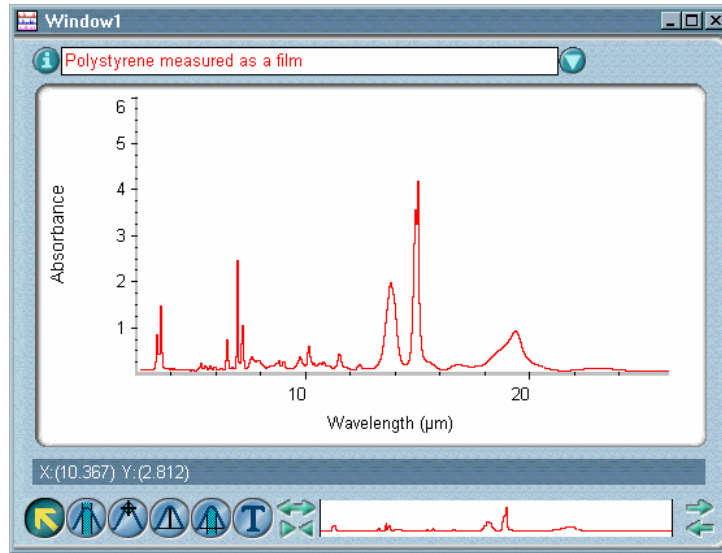
It is easier to see fine spectral details in this format than in other formats.



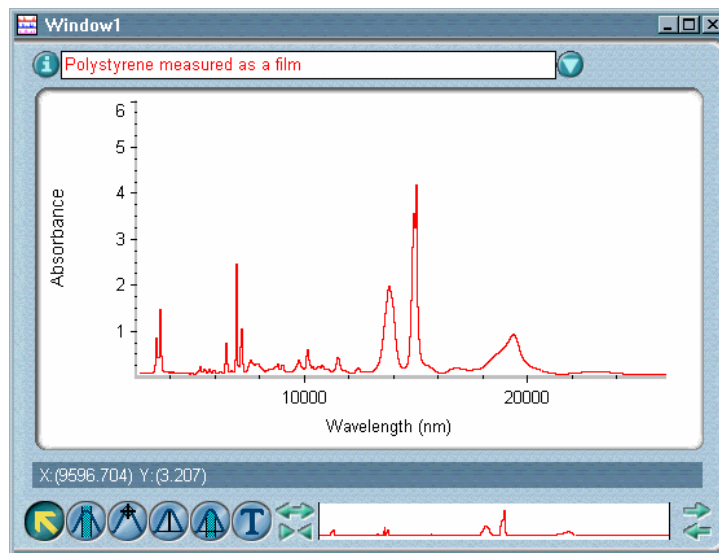
This format is suitable for high resolution and gas phase spectra. This format is used by the Aldrich spectral library books and is very helpful for spectral interpretation.

**Wavelength ( $\mu\text{m}$ )** – In this format (see the following example) spectra are displayed in wavelength measured in micrometers ( $\mu\text{m}$ ), and the default displayed spectral range for mid-IR data (4000 to 400 wavenumbers) is from 2.5 to 25 micrometers.

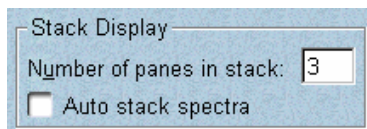
Mid-IR spectra are generally hard to interpret in this format, because their peaks are displayed too close together.



**Wavelength (nm)** – In this format (see the example below) spectra are displayed in wavelength measured in nanometers (nm), and the default displayed spectral range for mid-IR data (4000 to 400 wavenumbers) is from 2500 to 25000 nanometers.



## Specifying how to stack spectra



The options in the Stack Display box affect stacked spectra. Use Number Of Panes In Stack to specify the number of panes to display when you stack spectra using Stack Spectra in the View menu. Typically two panes are stacked for visually comparing spectra. This parameter is not available if Auto Stack Spectra is turned on.

Turn on Auto Stack Spectra if you want the number of panes in a stack adjusted automatically to match the number of displayed (not hidden) spectra instead of using the number specified by Number Of Panes In Stack. This lets you see every displayed spectrum in the window without using the stack scroll bar. Keep in mind, however, that the panes become smaller as you add spectra to the window.

**Note** You can specify how to stack spectra in newly created spectral windows by setting options in the Stack Display box in the Window options (available through Options in the Edit menu). See “Specifying how to stack spectra in new spectral windows” in the “Edit” chapter for details. ▲

See “Stacking or overlaying spectra” in this chapter and “Stacking spectra” in the “About the Display” chapter for more information on stacking spectra.

## Specifying the sampling information to display

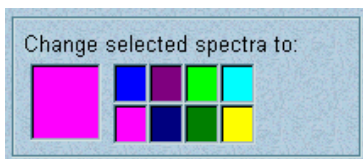
When the Sampling Information parameter is on (see “Displaying sampling information”), you can select from the Sampling Information box the following kinds of information to display. (Both the Sampling Information option and the desired items in the Sampling Information box must be turned on for sampling information to be displayed.) The information will be displayed for the most recently selected spectrum that is currently displayed in the spectral window or for all the displayed spectra in the window if they are stacked.

Information	Description
Company Name	Name entered when the software is installed.
Title Of Spectrum	Title of the displayed spectrum.
Date And Time	Date and time the spectrum was collected.
Data Collection:	
Sample Scans	Number of sample scans collected.
Background Scans	Number of scans collected for the background spectrum used to process the sample spectrum.
Resolution	Resolution used for sample and background data collection.
Gain	Gain used to amplify the detector signal.

Information	Description
Optical Velocity	A value that is twice the velocity of the moving mirror.
Aperture	Relative size of the aperture expressed as a percent of maximum area.
Bench Configuration:	
Detector	Type of detector used.
Beamsplitter	Type of beamsplitter used.
Source	Type of source used.
Accessories	Accessories used to collect the spectrum.
Comments	Any comments about the spectrum that you have recorded in the Collection And Processing Information window. See “Collection and processing information” in the “About the Display” chapter for details.
Filename	The filename of the spectrum.
System Status Results	The results of System Performance Verification tests, as shown in the Collection And Processing Information window.

**Note** You can specify the sampling information to display in newly created spectral windows by selecting options in the Sampling Information box in the Window options (available through Options in the Edit menu). ▲

## Selecting a color for the currently selected spectra



Use Change Selected Spectra To to specify a color for displaying the currently selected spectra whenever those spectra are not selected. There are eight color choices, which are determined by the current selections in the Colors dialog box in the View options. (See “Specifying colors for spectra and other features” in the “Edit” chapter for details on selecting these display colors.) The color you select will appear in the box to the left of the color choices.

When you exit the Display Setup dialog box, the currently selected spectra will still be in the color specified for selected spectra. When the spectra are no longer selected, they will be displayed in the color you specified.

**■ How to ➡**

Set the display parameters

- 1. Select the spectral window whose display parameters you want to set.**

If only one spectral window currently exists, that is the selected window.

- 2. If you want to select a color for displaying one or more spectra in the window, select the spectra.**

If you only want to set other display parameters, skip this step.

- 3. Choose Display Setup from the View menu.**

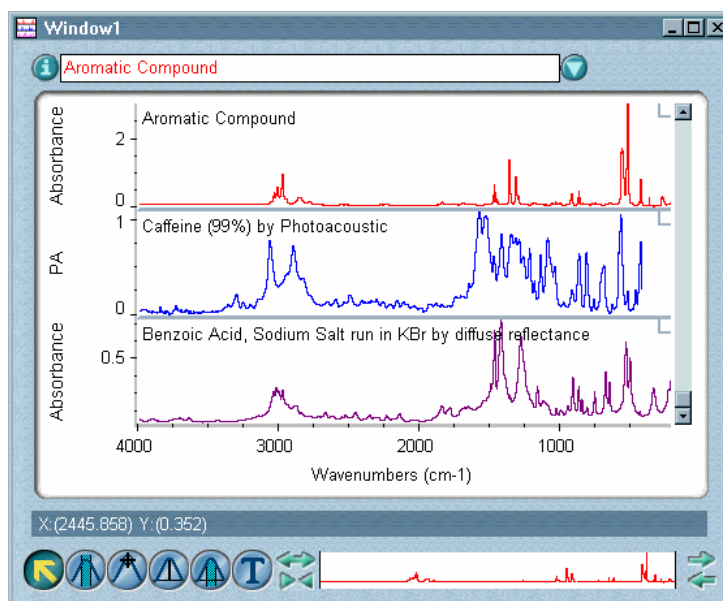
The Display Setup dialog box appears.

- 4. Set the parameters as desired.**

- 5. Choose OK.**

## Stacking or overlaying spectra

If the spectra in the active spectral window are currently overlaid, Stack Spectra is available in the View menu. When you choose the command, the spectra appear in a “stack” of panes, each of which can contain only one spectrum (see the following example), and the command name changes to Overlay Spectra.

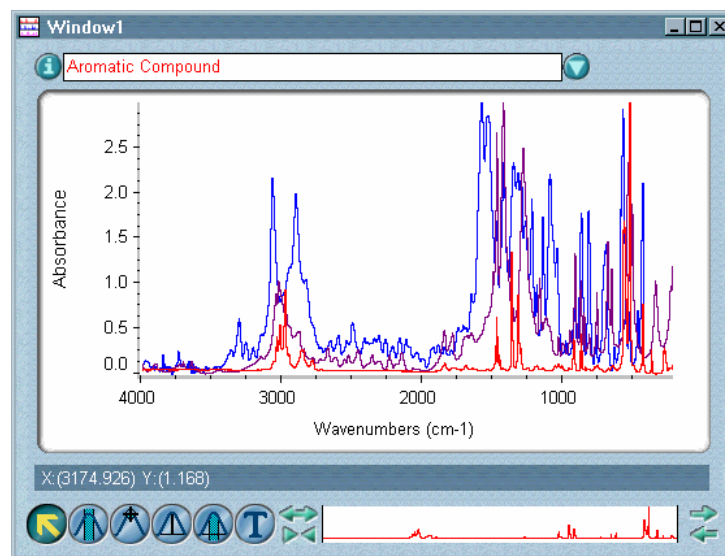


### Stacked spectra

Stacking spectra is most useful when you are comparing spectra that are significantly different. The number of stacked panes is determined by the setting of Number Of Panes In Stack or Auto Stack Spectra in the Stack Display box in the Display Setup dialog box. See “Specifying how to stack spectra” for details.

If the spectra are currently stacked, Overlay Spectra is available in the View menu. When you choose the command, the spectra are overlaid and the command changes to Stack Spectra. Overlaying spectra makes it easy to compare them visually, especially when their features are similar.

Here is an example:



## Overlaid spectra

For more information on overlaying and stacking spectra, see “Overlaying and stacking spectra” in the “About the display” chapter.

### — How to ➔

Stack or overlay spectra

#### 1. Select the spectral window that contains the spectra.

If only one spectral window currently exists, that is the selected window.

#### 2. Choose Stack Spectra or Overlay Spectra from the View menu.

## Hiding spectra

Use Hide Spectra in the View menu to hide the selected spectra from view. A hidden spectrum cannot be seen in the spectral window; only its title appears in the title box list. The title is displayed using the font specified for the titles of hidden spectra in the View options (available through Options in the Edit menu). The default font for displaying the titles of hidden spectra is italic. The order of titles is not affected when you hide a spectrum.

To make a hidden spectrum visible again, click its title in the title box list.

When you hide a selected spectrum, it is no longer selected. If any spectra remain in the window after you hide the selected spectra, one of the remaining spectra will be selected automatically.

**Note** If you hide an overlaid spectrum whose sampling information is displayed, the sampling information is removed from the screen. The sampling information for another selected spectrum is displayed if there is one displayed in the window. ▲

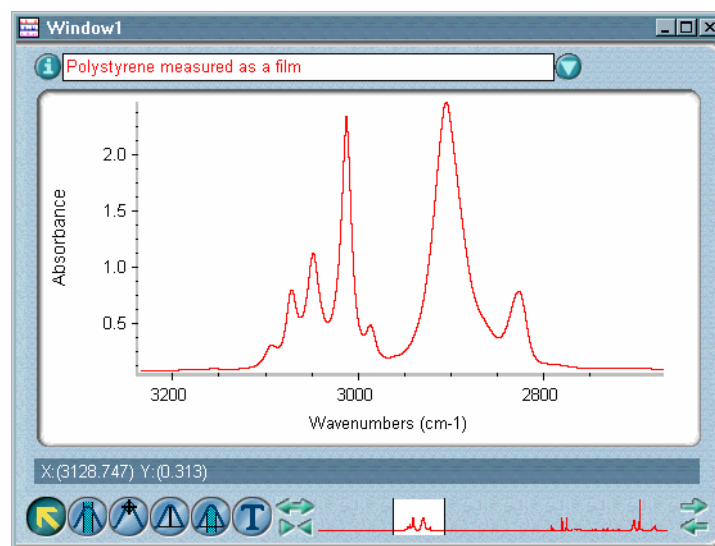
See “Stacking spectra” in the “About the Display” chapter for more information on hiding spectra.

— **How to** ➔ Hide a spectrum or spectra

1. **Select the spectra.**
2. **Choose Hide Spectra from the View menu.**

## Displaying spectra full scale

Use Full Scale in the View menu to adjust the vertical scale of the spectra in the active spectral window so that they fill their panes. If annotations are displayed, the spectrum’s vertical scale is adjusted as needed to keep any completely displayed annotations within view. (Labels not fully visible in the pane will not be taken into account when the scale is adjusted.) Here is an example:



Spectrum displayed full scale



Full Scale brings the highest data point of each spectrum (or the highest point of its annotations) to the top of the pane and the lowest data point of each spectrum (or the lowest point of its annotations) to the X-axis. (See “Displaying spectra full scale automatically” for information on displaying spectra full scale automatically.)

If there are peaks or annotations higher than the top of the pane or a baseline or annotation below the bottom of the pane or X-axis, Full Scale adjusts the vertical scale of the spectrum so that its baseline, peaks and annotations all fit in the pane.

Full Scale changes the vertical scale for the entire spectrum, not just the displayed portion. However, only the displayed region is used to find the highest and lowest points that will be used when the vertical scale is changed.

**Note** Since the Y-axis applies only to the selected overlaid spectrum, you will not see the change in the Y-axis for a non-selected, overlaid spectrum until it is selected. ▲

### ■ *How to* ➡

Adjust the vertical scale of spectra to fit their panes

#### 1. **Select the spectral window that contains the spectra.**

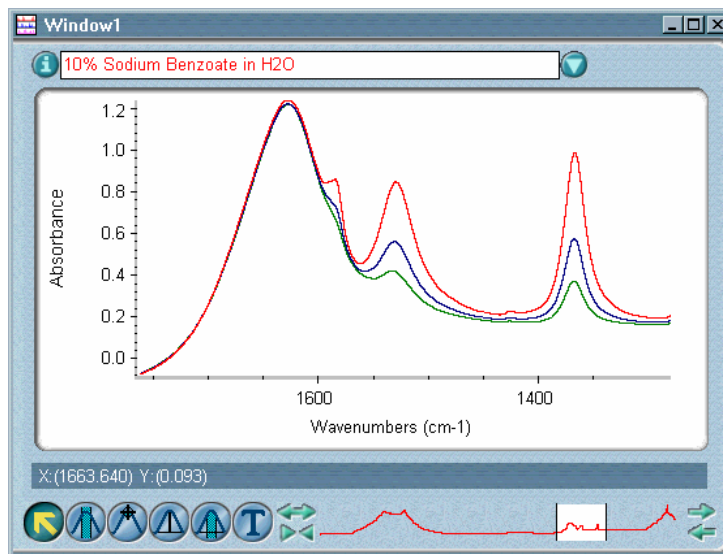
If only one spectral window currently exists, that is the selected window.

#### 2. **Choose Full Scale from the View menu.**

The spectra are displayed full scale, and a check mark appears next to the command name. If you change the Y-axis scale of the spectra, the check mark is removed.

## Displaying spectra using the same Y-axis

Use Common Scale in the View menu to display all the spectra in the active spectral window using the same Y-axis scale, making it easy to compare their relative peak heights visually. The minimum and maximum Y values from all the spectra become the new Y-axis display limits. See the following example.



Common Scale changes the display scale for the entire X-axis range, not just the displayed portion. However, only the displayed region is used to calculate the highest and lowest points which will define the common scale.

Displaying spectra with a common scale is useful when you are quantifying spectra or comparing them visually to see differences in the concentrations of components.

### — *How to* ➔

Display spectra using the same Y-axis

#### 1. Select the spectral window that contains the spectra.

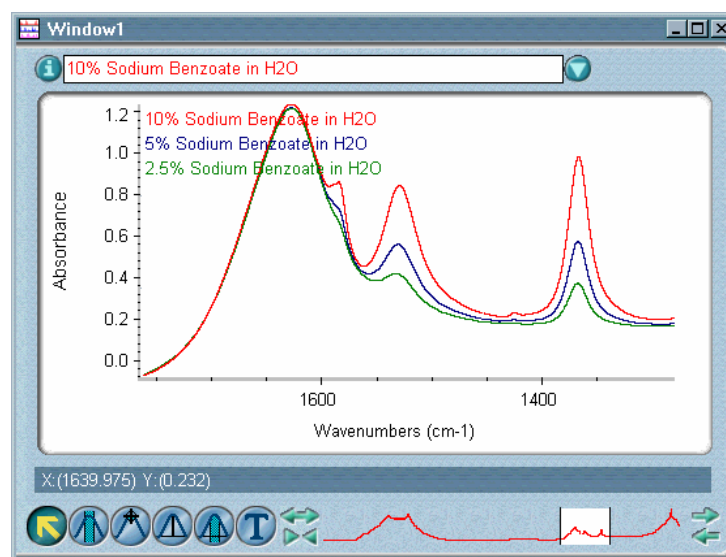
If only one spectral window currently exists, that is the selected window.

#### 2. Choose Common Scale from the View menu.

The spectra are displayed using the same Y-axis scale, and a check mark appears next to the command name. If you change the Y-axis scale of the spectra, the check mark is removed.

## Matching the Y scale of a spectrum

Use Match Scale in the View menu to display all the spectra in a spectral window using the minimum and maximum Y values of the selected spectrum as the Y-axis display limits. This makes it easy to compare their relative peak heights visually. See the following example.



### — How to →

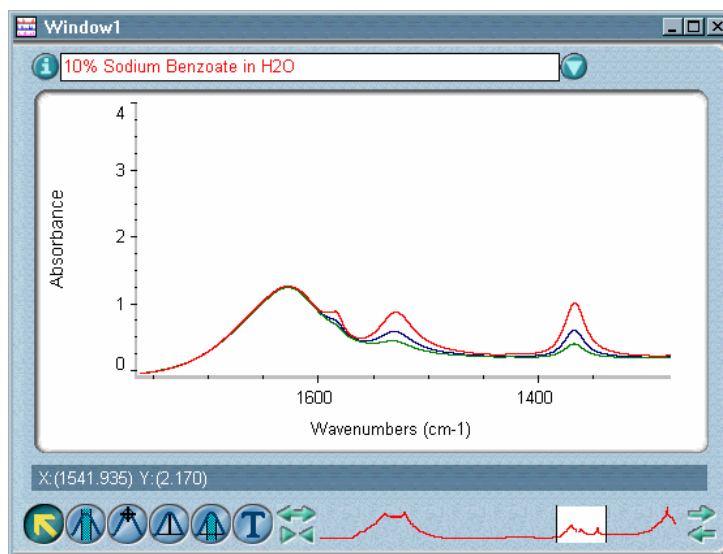
Match the Y-axis scale of a spectrum

1. **Select the spectrum.**
2. **Choose Match Scale from the View menu.**

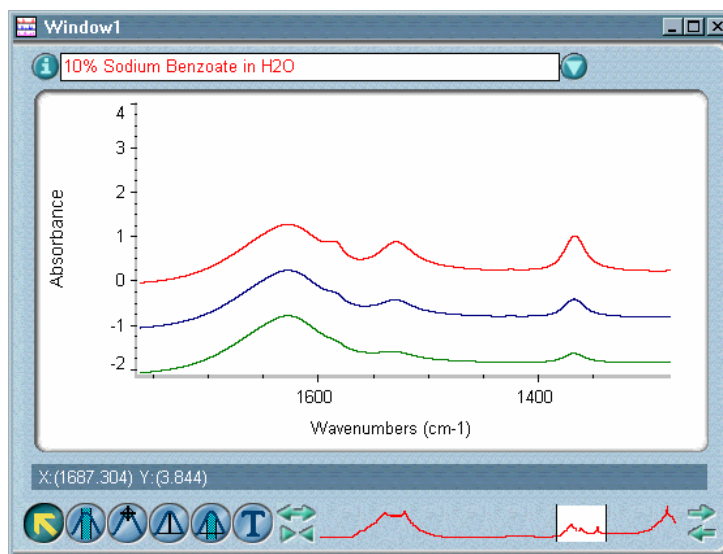
All the spectra in the window are displayed using the Y-axis limits of the selected spectrum, and a check mark appears next to the command name. If you change the Y-axis limits of the spectra, the check mark is removed.

## Displaying spectra vertically offset

If you are overlaying spectra, you can use Offset Scale in the View menu to display the spectra in the active spectral window vertically offset from each other. Separating the spectra in this way lets you compare their spectral features at any frequency. The following example shows three overlaid spectra.



Here are the same spectra after being offset:



Immediately after you choose Offset Scale, the Y-axis is accurate only for the selected spectrum. If you then select another spectrum in the window, the Y-axis becomes accurate for it.

Hidden spectra are not affected by Offset Scale.

**Note** If Offset Scale does not adequately separate the spectra, you can use the selection tool to drag the spectra up or down. ▲

**— How to ➡** Display spectra vertically offset

**1. Select the spectral window that contains the spectra.**

If only one spectral window currently exists, that is the selected window.

**2. Choose Offset Scale from the View menu.**

The displayed spectra are offset vertically on the screen, and a check mark appears next to the command name. If you change the Y-axis scale of the spectra, the check mark is removed.

## Setting the display limits

Use Display Limits in the View menu to specify the X-axis and Y-axis display limits for spectra in the currently active spectral window. The Y-axis limits apply only to the selected spectra unless you turn on Apply To All Spectra.

**Note** You can set the X-axis display limits for newly created spectral windows by setting options in the Window options. See “Specifying X-axis display limits for new spectral windows” in the “Edit” chapter for details. ▲

**— How to ➡** Specify the display limits

**1. Select the spectra whose Y-axis display limits you want to set. If you want to set the Y-axis display limits for all the spectra in a spectral window, just select the window and go to the next step.**

To select more than one spectrum in a spectral window using the selection tool, hold down the Control key when clicking the spectra.

**2. Choose Display Limits from the View menu.**

The Display Limits dialog box appears.

**3. Type the desired X-axis limits in the text boxes in the X-Axis Limits box.**

4. **Type the desired Y-axis limits in the text boxes in the Y-Axis Limits box.**
5. **If you want the new Y-axis limits to apply to all the spectra in the spectral window, turn on Apply To All Spectra.**

If this option is off, the Y-axis limits will apply to the selected spectra only.

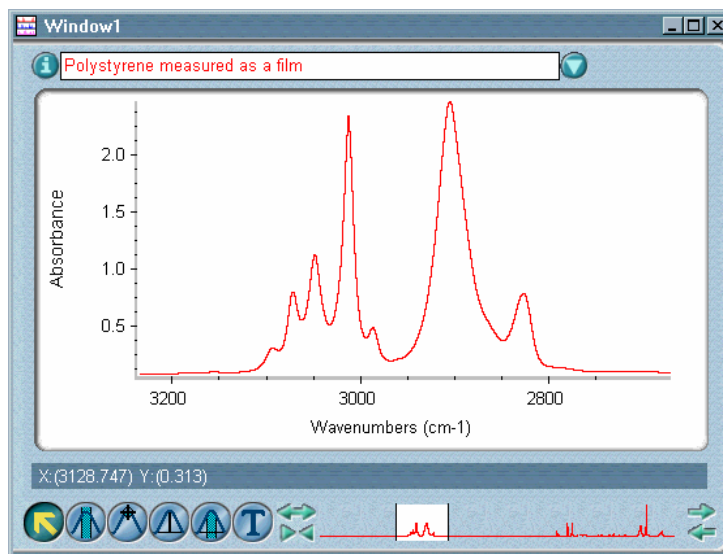
6. **Choose OK.**

The spectra are then displayed using the limits you specified.

## Displaying spectra full scale automatically

Automatic Full Scale in the View menu automatically displays the spectra in the active spectral window full scale whenever you display a different spectral region using the selection tool or view finder. This is useful when you always want to view your spectra full scale.

Automatic Full Scale brings the highest data point of each spectrum (or the highest point of its annotations) to the top of its pane and the lowest data point of each spectrum (or the lowest point of its annotations) to the X-axis. Here is an example:



If annotations are displayed for a spectrum, the spectrum's vertical scale is adjusted as needed to keep the annotations within view.

**Note** Turn off Automatic Full Scale if you want to be able to adjust the display of spectra so that they are not full scale. ▲

**— How to →** Display spectra full scale automatically

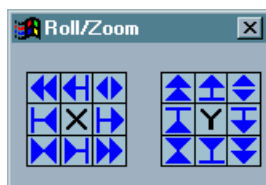
### **Choose Automatic Full Scale from the View menu.**

A check mark appears next to the command name when the command is on. As long as the command is on, spectra in the active spectral window will be displayed full scale when you display a different spectral region using the selection tool or view finder.

To turn the command off, choose Automatic Full Scale from the View menu when the check mark is present. The check mark is removed.











## **Rolling and zooming spectra**

Roll/Zoom Window in the View menu lets you access a set of symbols that you can use to adjust the display of spectra in the active spectral window. These symbols appear in the Roll/Zoom window.













The symbols in the group labeled “X” affect the X scale of displayed spectra; the symbols in the group labeled “Y” affect the Y scale.

The following table shows the effect of using each of these symbols. If you prefer, you can use the keys and key combinations on the numerical keypad listed in the table to roll or zoom spectra. The “Num Lock” feature on your keyboard must be turned off and the Roll/Zoom window must be displayed to use these keys. The Num Lock feature is turned off automatically when you display the window.

Symbol	Effect on Display	Keypad
	Moves all the spectra to the left (to view a spectral region to the right). This has the same effect as rolling your view to the right with the top half of the view finder's Roll button.	4
	Expands all the spectra horizontally while keeping the right edge of each spectrum in place.	3 + 4
	Expands all the spectra horizontally about the center of the pane. This has the same effect as using the top half of the view finder's Horizontal Expand/Contract button.	3
	Contracts all the spectra horizontally while keeping the left edge of each spectrum in place.	1 + 4
	Expands all the spectra horizontally while keeping the left edge of each spectrum in place.	3 + 6
	Contracts all the spectra horizontally about the center of the pane. This has the same effect as using the bottom half of the view finder's Horizontal Expand/Contract button.	1
	Contracts all the spectra horizontally while keeping the right edge of each spectrum in place.	1 + 6
	Contracts all the spectra horizontally while keeping the right edge of each spectrum in place.	1 + 6
	Moves all the spectra to the right (to view a spectral region to the left). This has the same effect as rolling your view to the left with the bottom half of the view finder's Roll button.	6
	Moves the selected spectrum up. (If multiple spectra are selected, only the first one selected is moved.)	8



Symbol	Effect on Display	Keypad
	Expands the selected spectrum vertically while keeping the bottom of the spectrum in place. (If multiple spectra are selected, only the first one selected is expanded.) This has the same effect as using the left half of the view finder's Vertical Expand/Contract button, except that all the selected spectra are expanded when you use the button.	8 + 9
	Expands the selected spectrum vertically about the center of the pane. (If multiple spectra are selected, only the first one selected is expanded.)	9
	Contracts the selected spectrum vertically while keeping the top of the spectrum in place. (If multiple spectra are selected, only the first one selected is contracted.)	7 + 8
	Expands the selected spectrum vertically while keeping the top of the spectrum in place. (If multiple spectra are selected, only the first one selected is expanded.)	9 + 2
	Contracts the selected spectrum vertically about the center of the pane. (If multiple spectra are selected, only the first one selected is contracted.)	7
	Contracts the selected spectrum vertically while keeping the bottom of the spectrum in place. (If multiple spectra are selected, only the first one selected is contracted.) This has the same effect as using the right half of the view finder's Vertical Expand/Contract button, except that all the selected spectra are contracted when you use the button.	2 + 7
	Moves the selected spectrum down. (If multiple spectra are selected, only the first one selected is moved.)	2

**Note** The symbols , , and  do not affect spectra whose entire X range is currently displayed. ▲

**Note** Only one spectrum moves on the screen while you rolling or zooming spectra, even if several spectra are selected. When you are finished, all the spectra in the window are adjusted for any change you made in the X dimension. ▲

**Note** You can also roll and zoom spectra by using the Roll, Horizontal Expand/Contract and Vertical Expand/Contract buttons at the ends of the view finder. See “View finder” in the “About the Display” chapter for details. ▲

■ **How to** ➡ Roll and zoom spectra

**Choose Roll/Zoom Window from the View menu.**

The Roll/Zoom window appears and you can begin to roll or zoom spectra in the active spectral window. You can move the Roll/Zoom window to any part of the screen by dragging its title bar.

A check mark appears next to the command name in the View menu when the window is displayed. To remove the Roll/Zoom window from the screen, choose Roll/Zoom Window again or click the window’s Close button.

## Displaying and using a toolbar

Use Toolbar in the View menu to display a toolbar containing buttons that you can use to initiate commands, macros or external programs. The toolbar appears near the left side, top or right side of the OMNIC window, depending on the setting of Toolbar Location in the Edit Toolbar dialog box (available through Edit Toolbar in the Edit menu). If the specified buttons do not all fit in one column or row in the OMNIC window, additional columns or rows are used.

The image or text on each button represents the action taken by the 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 using the left mouse button.

The buttons included in the toolbar depend on the current software configuration. To create your own custom toolbar and save it with your configuration, use Edit Toolbar in the Edit menu and Save Configuration As in the File menu. See “Customizing a toolbar” in the “Edit” chapter and “Saving a configuration” in the “File” chapter for more information.

**■ How to ➔**

Display a toolbar

**Choose Toolbar from the View menu.**

A check mark appears next to the command name in the View menu when the toolbar is displayed. To remove the toolbar from the screen, choose Toolbar again.



# Process

The Process menu includes commands that let you perform these operations:

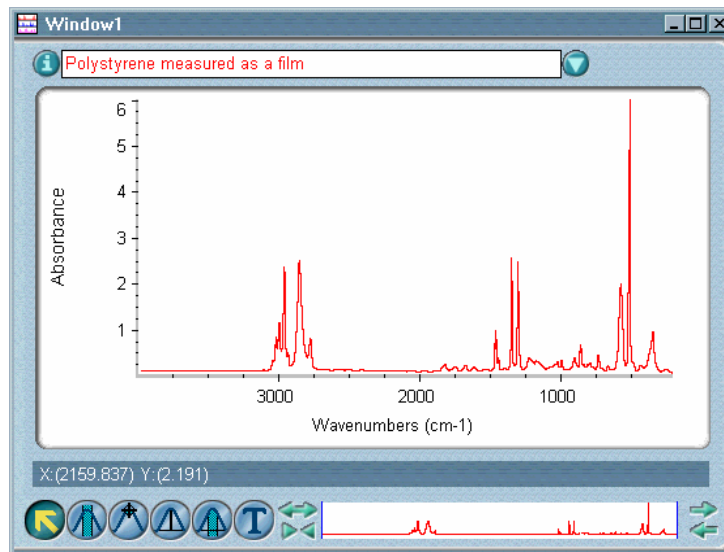
To do this...	Use this command...
Convert a spectrum to absorbance.	Absorbance
Convert a spectrum to % transmittance.	% Transmittance
Convert a spectrum to Kubelka-Munk, photoacoustic, % reflectance, log (1/R) or delta absorbance units or to wavenumbers, micrometers or nanometers.	Other Conversions
Fourier transform interferogram data.	Reprocess
Display the interferograms saved with the selected spectrum.	Retrieve Interferograms
Improve the baseline of a spectrum.	Baseline Correct
Improve a baseline automatically.	Automatic Baseline Correct
Correct ATR spectra for the shifting of infrared absorption bands and the effects of variation in depth of penetration.	Advanced ATR Correction
Correct photoacoustic data to enhance the infrared signal at the sample surface or improve quantitative linearity.	PAS Linearize
Convert a specular reflection spectrum to a transmission spectrum and produce refractive index and absorption index plots.	Interactive Kramers-Kronig
Correct spectra for variations in the depth of penetration or for water or carbon dioxide absorptions or convert a specular reflection spectrum to a transmission spectrum.	Other Corrections
Erase a spectral region.	Blank

To do this...	Use this command...
Replace a spectral region with a straight line.	Straight Line
Subtract one spectrum from another.	Subtract
Subtract a component from a spectrum.	Automatic Region Subtract
Separate overlapping spectral features.	Fourier Self-Deconvolution
Smooth sharp peaks in a spectrum.	Smooth
Smooth sharp peaks in a spectrum automatically.	Automatic Smooth
Change the data point spacing of a spectrum.	Change Data Spacing
Convert a spectrum to its first or second derivative.	Derivative
Multiply a spectrum by a number.	Multiply
Add two spectra together.	Add
Perform arithmetic operations on spectra.	Spectral Math
Normalize the laser frequency of a spectrum.	Normal Frequency
Normalize the Y-axis scale of a spectrum.	Normalize Scale

You can customize the way OMNIC processes data by setting options using the Options command in the Edit menu. See “Customizing OMNIC by setting options” in the “Edit” chapter for details.

## Converting spectra to absorbance

Use Absorbance in the Process menu to convert spectra to absorbance units (see the example below). Absorbance units show the amount of infrared energy absorbed by the sample.



The absorbance scale is useful in many areas of spectral analysis. You should normally convert spectra to absorbance before performing these tasks:

- Quantitative analysis. Since absorbance varies linearly with concentration in most cases, it is the basis of all FT-IR quantitative analysis.
- Subtracting one spectrum from another.
- Correcting the baseline of a spectrum.
- Searching a spectral library to identify an unknown spectrum (qualitative analysis).

Absorbance at a frequency is defined by the equation

$$A = \log(100/\%T)$$

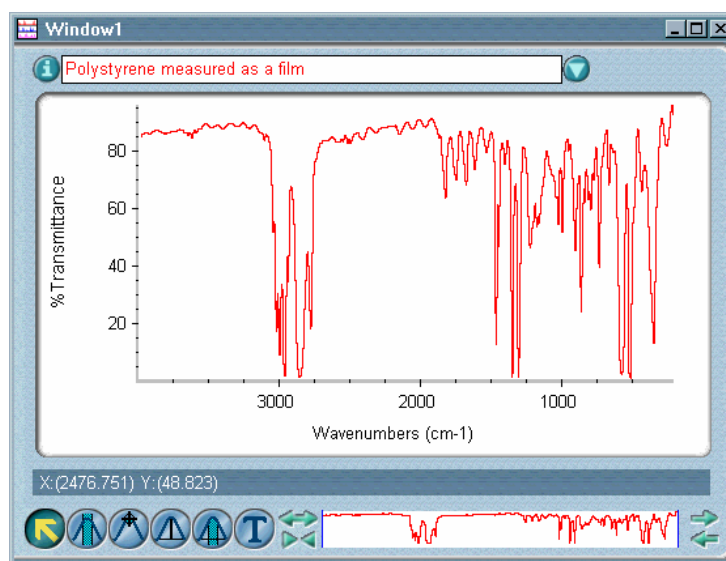
where %T is the percent transmittance value.

— **How to** ➔ Convert spectra to absorbance

1. **Select the spectra.**
2. **Choose Absorbance from the Process menu.**

## Converting spectra to % transmittance

Use % Transmittance in the Process menu to convert spectra to % transmittance units (see the following example). These units show the relative amount of infrared energy transmitted through the sample.



For historic reasons published infrared reference spectra are generally presented in % transmittance. It is easier to compare spectra qualitatively when they are presented using the same Y-axis format. The % transmittance format is generally not as good as absorbance for manipulating data and performing quantitative analyses.

Percent transmittance at a frequency is defined by the equation

$$\%T = (S/B) * 100$$

where S is the intensity of infrared energy through the sample and B is the intensity of infrared energy without a sample in place. B is called the background.



— **How to** ➔ Convert spectra to % transmittance

1. **Select the spectra.**
2. **Choose % Transmittance from the Process menu.**

## Converting spectra to special units

Use Other Conversions in the Process menu to convert spectra to the following units.

*Y-axis units:*

- Kubelka-Munk units
- photoacoustic units
- % reflectance units
- log (1/R) units
- delta absorbance

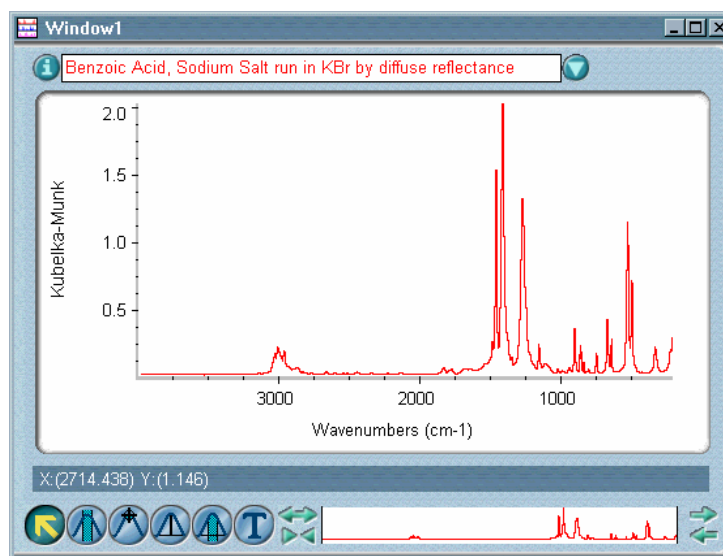
*X-axis units:*

- wavenumbers
- micrometers
- nanometers

The units are described in the next sections.

## Kubelka-Munk

Select Kubelka-Munk to convert % reflectance spectra collected using the diffuse reflection (DR) technique to Kubelka-Munk units (see the following example). Since these units are similar to absorbance units, the Kubelka-Munk format is useful for searching diffuse reflectance spectra against absorbance spectra in commercially available libraries. (Kubelka-Munk spectra are actually searched in absorbance.)



Because of pathlength variation, in many cases the concentration of samples run using the diffuse reflection technique do not vary linearly with  $\log(1/R)$  (which is the equivalent of absorbance for reflection measurements). The Kubelka-Munk scale was developed to provide a more linear relationship with respect to concentration.

When you develop quant methods for determining component concentrations in sample mixtures, you can use spectra in  $\log(1/R)$  or Kubelka-Munk units. Kubelka-Munk units are normally preferred because they eliminate any wavelength-dependent specular reflection effects, which reduce the accuracy of the analysis.

However, the Kubelka-Munk model is accurate only if these criteria are met:

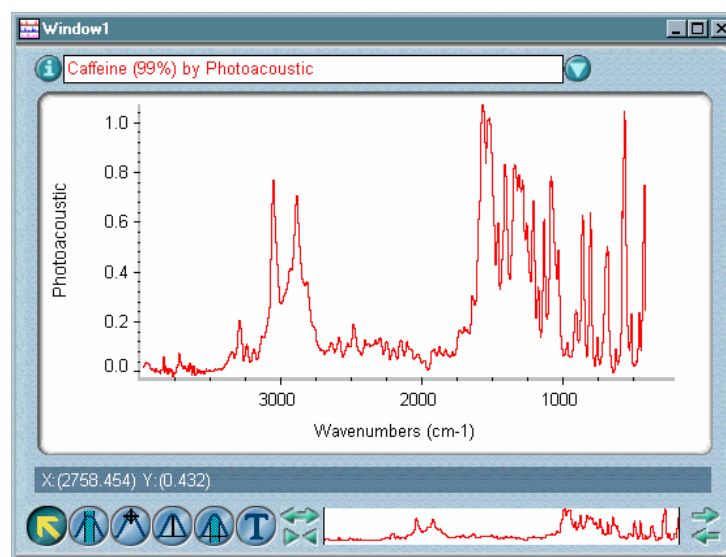
- You are using high quality DR spectra.
- The sample is diluted with a nonabsorbing matrix material such as KBr.
- The sample concentration is low (about 1% sample to 99% matrix by weight).
- The sample and matrix material are finely ground (a particle size of 2 to 5 micrometers is recommended).
- The mixture is uniform in particle size and composition.
- The sample thickness must be at least 3 mm.

If these criteria are not met, use  $\log(1/R)$  units instead of Kubelka-Munk, or see which scale gives a more linear response.

The Kubelka-Munk value at a frequency is defined by the equation  $KM = (1 - R)^2/2R$ , where R is the reflectance intensity of the sample divided by the reflectance intensity of the standard.

## Photoacoustic

Select Photoacoustic to convert spectra collected using a photoacoustic technique to photoacoustic units (see the following example). Spectra in these units resemble absorbance spectra and can be searched against a library of absorbance spectra.



In a photoacoustic experiment the intensity of the incident light is modulated at a frequency in the acoustic range. The sample absorbs the light energy, which is converted into heat. This causes intermittent thermal expansion of the sample and the adjacent media, producing a sound wave that travels to an acoustic transducer. The transducer converts the sound into an electrical signal, which is processed to produce a spectrum.

The photoacoustic technique produces a spectrum that is more like a spectrum from an emission technique than a spectrum from a transmission technique. Thus, bands appear to be inverted when viewed using the % transmittance scale.

Converting the spectrum to photoacoustic units does three things:

- It identifies the sampling technique.
- It indicates which type of spectral library to use to identify the spectrum.

- By inverting the peaks, it makes the spectrum transmission-like. This lets you use the spectrum in a subtraction operation with another transmission-like spectrum or search the spectrum against a library of transmission-like spectra.

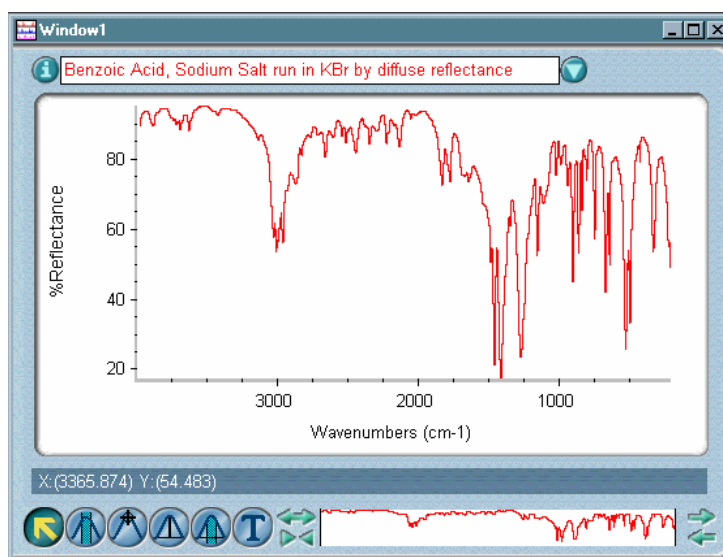
The photoacoustic value (PAS) at a frequency is defined by the equation

$$\text{PAS} = 100(I_S/I_B)$$

where  $I_S$  is the intensity of energy emitted as thermal waves by the sample and  $I_B$  is the intensity of energy emitted by the background material (usually carbon black). (Numerically, this is identical to % transmittance.)

## % Reflectance

Select % Reflectance to convert spectra collected using a reflection technique to % reflectance units (see the following example). These units show the amount of infrared energy reflected from the sample. Some common reflection techniques include diffuse reflection (DR) and specular reflection (SR).



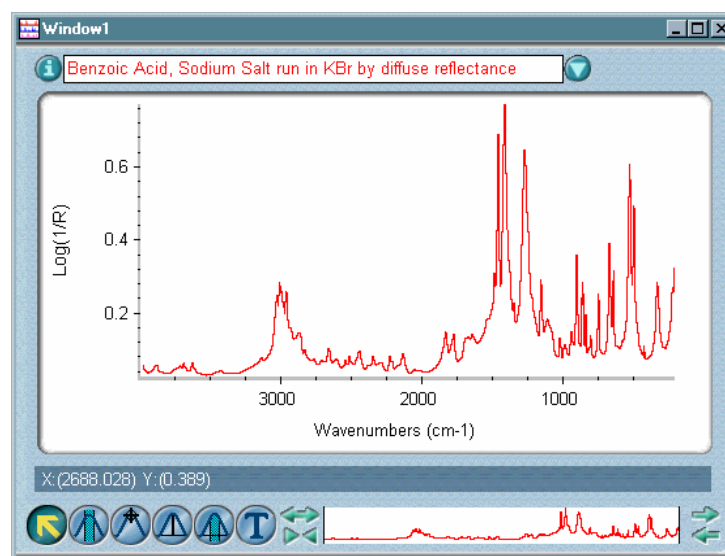
Percent reflectance at a frequency is defined by the equation

$$\%R = (I_S/I_B)*100$$

where  $I_S$  is the intensity of infrared energy reflected from the sample and  $I_B$  is the intensity of infrared energy passing through the reflection accessory with the sample replaced by a reference sample, usually a mirror for SR, powdered potassium bromide (KBr) or chloride (KCl) for DR, or simply the open crystal for ATR.  $I_B$  is called the background.

## Log (1/R)

Select Log (1/R) to convert reflection spectra to log (1/R) units (see the following example). These units show the amount of infrared energy absorbed by the sample in a reflection experiment. You can convert spectra collected using the specular reflection (SR) and diffuse reflection (DR) techniques. Displaying these spectra in log (1/R) units is useful for identifying the technique used to obtain the data.



The log (1/R) value at a frequency is defined by the equation

$$\log (1/R) = \log (100/\%R)$$

where %R is the % reflectance value of infrared energy at the same frequency. Displaying a reflectance spectrum in log (1/R) units is useful because there is often a linear relationship between the concentration of a component in a sample and the measured log (1/R) value.

Log (1/R) for reflection measurements is equivalent to absorbance in transmission measurements.

## Delta absorbance

Select DeltaAbsorbance to convert step-scan, time-resolved, single-beam spectra to delta absorbance spectra. This manual operation lets you carefully examine data before processing it, helping you to understand and optimize the data collection parameters for challenging TRS experiments. The data you process must have been collected and saved as single-beam data, or reprocessed and saved as single-beam data.

The conversion applies the following operation to the original data:

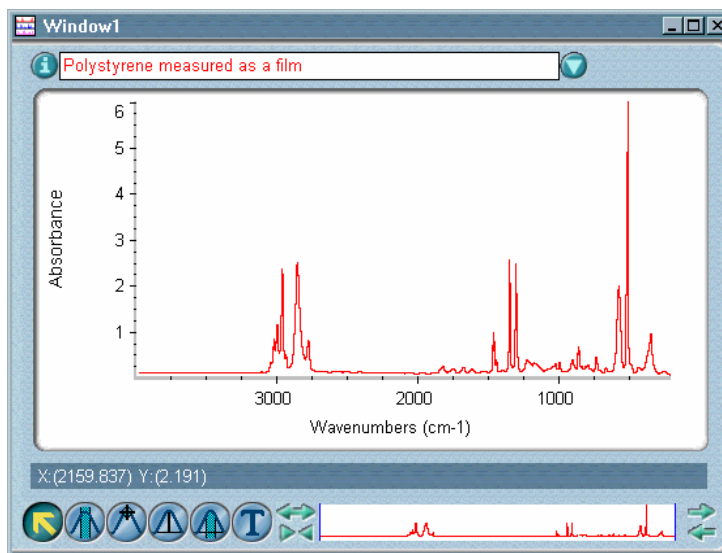
$$S' = -\log (1 + S/R)$$

where S is the selected spectrum, R is the static single-beam spectrum from the step-scan, time-resolved data collection, and S' is the resulting delta absorbance spectrum.

**Note** The delta absorbance calculation is valid only when the dynamic TRS single-beam spectra are uncoupled to detector DC output; that is, the data must have been collected with Add Static IFG To TRS IFGs not selected in the Step-Scan Time-Resolved Data Collection dialog box (available through the optional SST menu). ▲

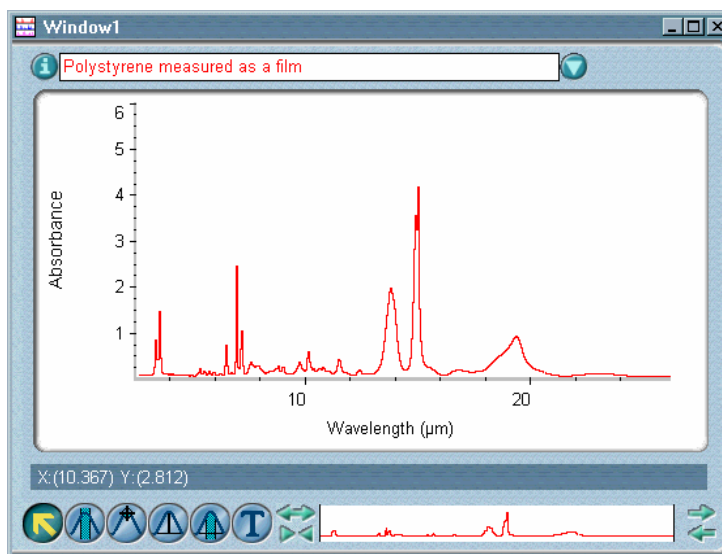
## Wavenumbers

Select Wavenumbers to convert spectra in wavelength (such as JCAMP-DX spectra) to wavenumbers (see the following example). A wavenumber is the number of waves per centimeter (the inverse of wavelength) and is the most commonly used X-axis unit. Use wavenumbers to display mid-IR and far-IR spectra.



## Micrometers

Select Micrometers to convert spectra in wavenumbers to micrometers (see the following example). A micrometer equals  $1 \times 10^{-6}$  meter and is the X-axis unit normally used for displaying infrared spectra in wavelength.

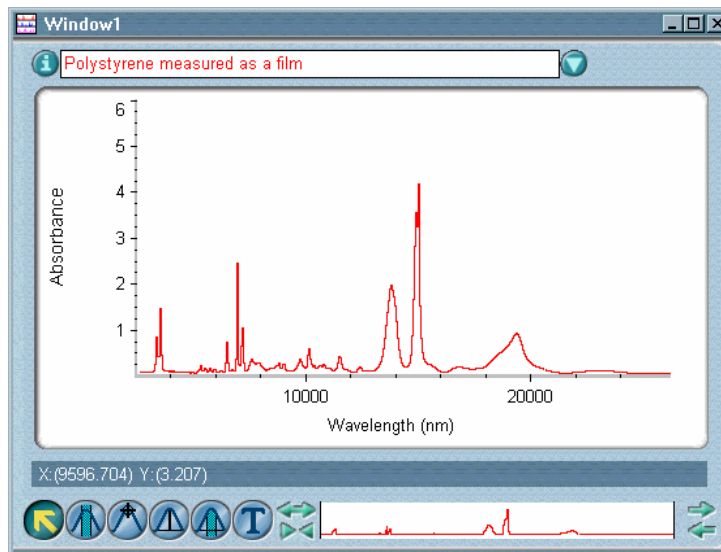


Micrometers were used more commonly in the past. Convert a spectrum to micrometers if you want to compare it visually with other data in micrometers.

## Nanometers

Select Nanometers to convert spectra in wavenumbers to nanometers. A nanometer equals  $1 \times 10^{-9}$  meter and is an X-axis unit used for displaying spectra in wavelength. Here is an example:

Use nanometers to display near-IR spectra.



### — *How to* ➔

Convert spectra to special units

1. **Select the spectra.**
2. **Choose Other Conversions from the Process menu.**

The Other Conversions dialog box appears.

3. **Select a conversion from the drop-down list box and then choose OK.**
  - If you selected Kubelka-Munk, Photoacoustic, % Reflectance or Log (1/R) units, the spectra are displayed using the selected Y-axis units and the procedure is finished.
  - If you selected DeltaAbsorbance, the Select Static Single-Beam Spectrum dialog box appears. Go to the next step.
  - If you selected Wavenumbers, Micrometers or Nanometers, a dialog box asks you to specify the data spacing of the data points. Go to step 5.



**4. Locate and select the desired single-beam spectrum and then choose Open.**

The converted data appears in the active window and the procedure is finished.

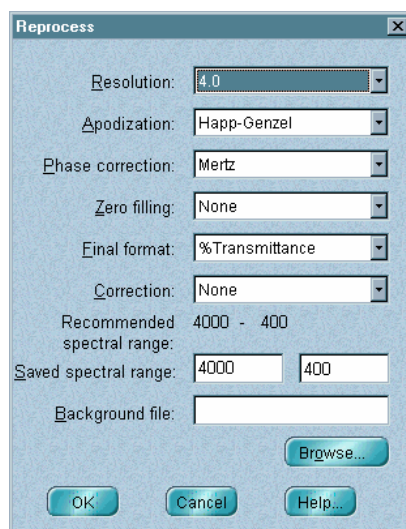
**5. Select the desired data spacing from the drop-down list box and then choose OK.**

**Note** If a spectrum is already displayed using the selected X-axis unit, it is not affected by this command. If you want to change the data spacing of the spectrum, use Change Data Spacing in the Process menu. ▲

The converted spectra are displayed using the selected X-axis unit and data spacing.

## Reprocessing spectra

Use Reprocess in the Process menu to transform the interferogram data for the selected spectra using different transformation parameter settings or ratio the spectra against a different background to improve the final data. You can use any background spectrum with saved interferograms stored on the disk and change the settings of any of the parameters in the Reprocess dialog box:



The sample and background interferograms must have been saved when the spectrum was collected to reprocess the data. Also, if you reprocess more than one spectrum at a time, all of them must have the same format (units) and resolution.

When the spectra are reprocessed, any spectral regions that were blanked or replaced with a straight line are restored.

**Note** You cannot reprocess a spectrum that was the result of a reprocessing operation. ▲

### **When to reprocess spectra**

It is sometimes desirable to change the way spectra have been calculated or manipulated, particularly when you are comparing several spectra. Here are some examples of when to use Reprocess to make such changes:

- To match parameter settings for quantitative analysis. In this type of analysis most of the parameters of the unknown spectrum must match those of the calibration standards used to create the method. If the parameters of an unknown are set incorrectly, you can often use Reprocess to match the settings without rerunning the sample.
- To match the resolution. If you want to compare a sample to other samples that were run at a lower resolution, you can reprocess the sample to that resolution.
- To match the apodization. Since apodization affects the “visual resolution” of spectra, reprocessing spectra to match their apodization types lets you compare them on an equal basis.
- To match the zero filling. Zero filling, along with resolution, determines the data point spacing, which is critically important when you use quantitative analysis methods. Reprocess lets you increase or decrease the number of levels of zero filling of a sample spectrum to match a quant method.
- To change the final format. You can use Reprocess to change the final format of spectra so that they have the same Y-axis units. (You can also do this with Absorbance, % Transmittance and Other Conversions in the Process menu.)

- To finish the processing of sample single-beam spectra or interferograms. This produces ratioed sample spectra.
- To change the correction type. This is most often used to “uncorrect” a spectrum stored on a disk. For example, you may have used Other Corrections in the Process menu to perform a Kramers-Kronig transformation on a spectrum and later realized that this was not appropriate.
- To change the spectral range. You may have saved data from 8,000 to 400  $\text{cm}^{-1}$  but later found that only the data from 1,800 to 700  $\text{cm}^{-1}$  are useful. Reprocessing with the smaller range will save disk space. In another case, you might find that you have lost useful data by saving too small a range; you can correct this by reprocessing with a larger saved range.
- To return to the original collected data for a spectrum.
- To improve the signal-to-noise ratio (SNR). Reprocessing a spectrum using a higher setting of Resolution (lower spectral resolution) can improve the SNR of the spectrum (although there can be a loss of important spectral information).
- To improve the data for an experiment by changing one or more parameters.

### ■ *How to* ➡

Reprocess a spectrum

- 1. Select the spectra.**
- 2. Choose Reprocess from the Process menu.**

The Reprocess dialog box shows the current settings of the transform parameters.

- 3. If you want to change the setting of a parameter, select a setting from the drop-down list box to the right of the parameter name.**

You can select a resolution that is less than or equal to that of the original spectra.

4. **If you want to reprocess the spectrum using a different background, choose Browse.**

In the dialog box that appears select a background file from any available directory or drive and then choose OK.

5. **When the parameters and background file are set the way you want them, choose OK.**

## Retrieving the interferograms saved with a spectrum

Use Retrieve Interferograms in the Process menu to display the interferograms for the selected spectrum in the active spectral window. To be retrieved and displayed, the interferograms must have been saved when the spectrum was collected. (You can use Experiment Setup to specify that interferograms be saved with spectra.)

The interferogram is the original measured data for a spectrum. If you discover a problem with the transformed data, you may be able to diagnose the problem by examining the interferogram. For example, a sine wave in the baseline of a spectrum usually indicates a “double pass” of the infrared beam through the sample. The corresponding interferogram will often show a “spike” on the side of the data. If you eliminate the spike (by using Straight Line in the Process menu), you can then reprocess the interferogram to eliminate the sine wave (by using a different background spectrum specified with the Browse button in the Reprocess dialog box).

### — *How to* ➔

Retrieve interferograms

1. **Select the spectrum.**
2. **Choose Retrieve Interferograms from the Process menu.**

The interferograms are displayed in the active spectral window. Both the sample and background interferograms appear if they are available. The titles of the interferograms are the same as the original spectrum title, with “Sample IFG” or “Background IFG” added at the end.

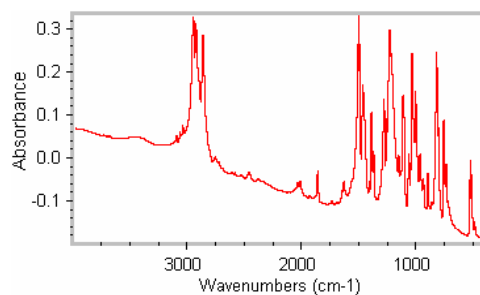
## Correcting a baseline manually

Use Baseline Correct in the Process menu to correct a sloping, curving, shifted or otherwise undesirable baseline of a spectrum so that the baseline appears flat and near zero absorbance units (or 100% transmittance). You can correct the baseline of a spectrum with any Y-axis units, but it is usually easier to select baseline points and see changes if the spectrum is in absorbance (or Kubelka-Munk or log (1/R) units) rather than in % transmittance (or % reflectance). Use Absorbance in the Process menu to convert a spectrum to absorbance. After the correction you can use % Transmittance or Other Conversions to convert the spectrum to its original units.

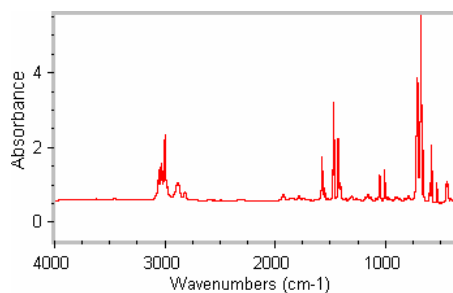
**Note** When you use this command, you specify the baseline points for the correction. If a baseline just has a simple tilt without other undesirable characteristics, you can use Automatic Baseline Correct to correct the baseline automatically, with the baseline points selected by the software. See “Correcting a baseline automatically.” ▲

## What is a baseline?

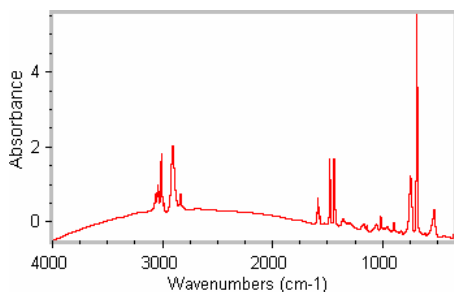
A baseline consists of the portions of a spectrum with no significant absorptions. Ideally the intensity in these portions is zero absorbance units (or 100 %T). In reality baselines may be tilted, shifted or curved (see the following examples).



### Tilted baseline



### Shifted baseline



### Curved baseline

## Why isn't a baseline always flat and at zero absorbance?

A baseline is affected by the quality of the background spectrum, the quality of the sample, the way the sample was prepared and the type of accessory that was used. Here are some examples of things that can cause baseline problems:

- A solid sample you run as a KBr pellet may exhibit scattering, especially if you did not grind the sample and KBr well enough before pressing the pellet. Large particles (greater than 5 micrometers) cause scattering. This results in increasing absorbance with higher frequency and is usually seen as an upward slope.
- The baseline may be well above zero absorbance if a pellet is too thick or the throughput of the sample and background measurements varies significantly.
- The absorbance values in an ATR spectrum may slope upward toward lower frequencies, because the depth of penetration into the sample increases and more energy is lost by reflection.
- The overall baseline of a spectral subtraction result may not be near zero absorbance if the baseline of the reference spectrum is significantly different from that of the sample spectrum.

## What are the benefits of correcting baselines?

You can obtain better results from searching spectral libraries, subtracting spectra or finding peaks if you first correct the baselines of your spectra. When you search a library, the entire sample spectrum—including baseline regions—is compared with the library spectra. If the spectrum's baseline is not flat and at zero absorbance (or 100 %T), the baseline regions will be considered to be significantly different from those of the library spectra. These differences will affect the search results.

Similarly, when you subtract a reference spectrum from a sample spectrum, the baseline regions are subtracted along with the regions that contain peaks. If the sample spectrum's baseline is not flat and at zero absorbance (or 100 %T), the baseline of the subtraction result will have the same undesirable characteristics. If you correct the baseline first, you can obtain a "clean" subtraction in which corresponding peaks are subtracted out, without baseline problems in the result.

When you use Find Peaks in the Analyze menu to locate peaks above a specified Y value, peaks "riding" on a baseline that is not flat and at zero absorbance (or 100 %T) may be found even though their corrected peak heights are less than the threshold. By correcting the baseline first, you can find peaks in a more consistent manner; that is, based on their height measured from the baseline.

A flat baseline is also helpful when you are visually comparing spectra or performing quantitative analysis.

When you add a spectrum to a user library, any negative absorbance values are set to zero by the normalization process. If you don't want those values set to zero, correct the baseline before adding the spectrum to the library.

Use Baseline Correct to correct a baseline by specifying the baseline points or Automatic Baseline Correct to correct a baseline with the baseline points selected automatically by the software.

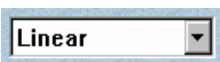
## **Using the baseline correction features**

Correcting a baseline manually involves clicking points on (or near) the baseline of the original spectrum displayed in the upper pane of the Baseline Correct window. As you move the pointer to the point you want to click, the readout below the panes shows the X and Y values of the pointer location. When you click a point, its Y value is subtracted from the Y value of the corresponding point in the spectrum to produce the new baseline point. The result is displayed in the lower pane. If you click a point directly on the baseline, that point will be brought to zero absorbance units (or 100 %T). By selecting points carefully, you can correct the baseline without clicking a large number of points.

In general, you should click points at the beginning and end of baseline regions that need to be corrected and “low points” above zero absorbance (or high points below 100 %T). When the clicked points are brought to zero absorbance (or 100 %T), the points between the clicked points will also be shifted so that their vertical position relative to the nearest clicked points is maintained.

**Notice** Be careful not to introduce false peaks or other inaccuracies when you click points. ▲

Similarly, if you click low points on both sides of a peak, the Y value of the peak will decrease but the peak height measured from the low points will stay the same.



Select the algorithm you want used for the baseline correction from the drop-down list box near the upper-left corner of the window. The algorithm determines how the software calculates the value to be subtracted from each data point in the spectrum to correct the baseline. The following table describes the available algorithms.

Algorithm	Description
Linear	A linear interpolation between specified baseline points is used. Use this algorithm for tilted or elevated baselines.
Spline	A cubic polynomial interpolation based on groups of four consecutive specified baseline points is used. Use this algorithm for curved baselines.
Polynomial	A polynomial that best fits all the specified baseline points is used. The order of the polynomial increases with the number of baseline points and has a maximum of six. Use this algorithm for S-shaped or severely distorted baselines.

You can use the buttons to the left and right of the panes to adjust the display of data for better viewing. To move the spectrum in the upper pane up or down, click the up arrow button or down arrow button, respectively.

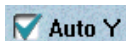


To expand a spectrum vertically, click the Expand button.



To contract a spectrum vertically, click the Contract button.





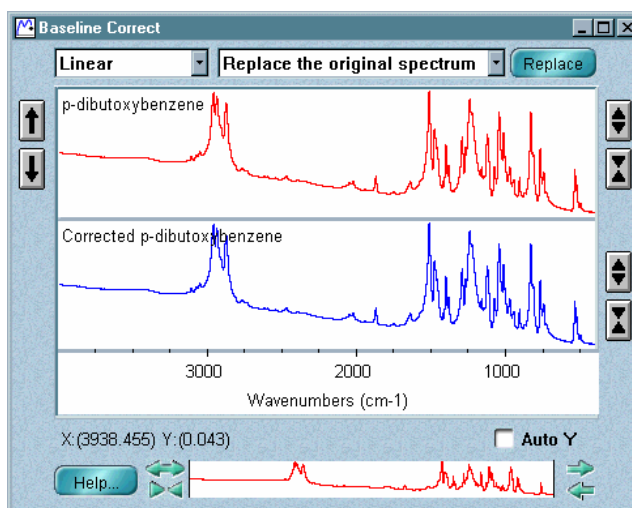
If you want your baseline points to coincide with points on the spectrum, turn on Auto Y. Each time you specify a baseline point by clicking, the point will be “snapped” to the spectrum. Any baseline points you specified with Auto Y turned off will also be snapped to the spectrum. This reduces the need to drag baseline points to obtain the best baseline correction.

### — How to —>

Correct a baseline manually

1. **Select the spectrum.**
2. **Choose Baseline Correct from the Process menu.**

The Baseline Correct window appears.

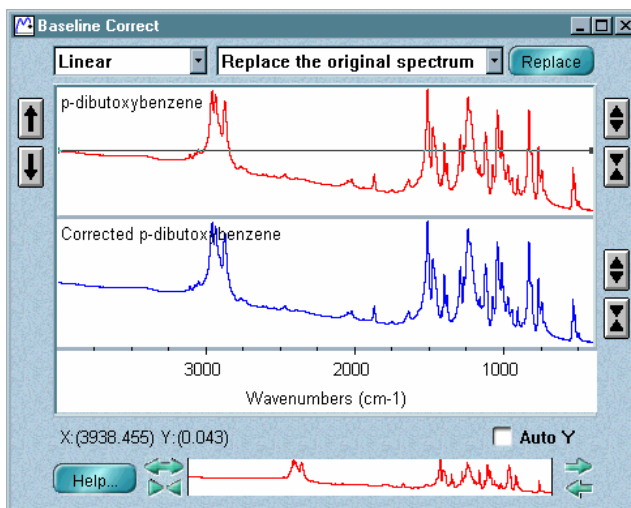


This window contains two panes; the entire original spectrum is displayed in the upper pane, and a duplicate image of the spectrum is displayed in the lower pane. As you correct the baseline in the upper pane, the corrected result is displayed in the lower pane.

3. **Select the desired algorithm from the drop-down list box near the upper-left corner of the window.**
4. **If you want your baseline points to coincide with points on the spectrum, turn on Auto Y.**

5. In the upper pane click the first point of the baseline that you want corrected.

A horizontal line is drawn through the baseline point you clicked. See the following example.



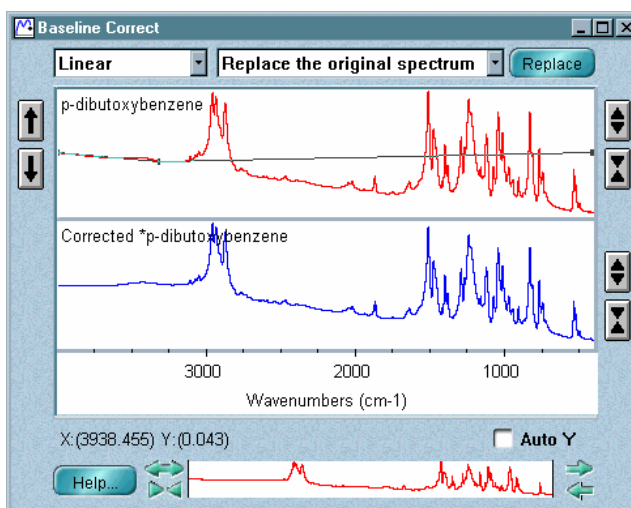
The X and Y values of the point appear below the lower pane.

**Note** If you are correcting the baseline of a spectrum on which you plan to perform a Kramers-Kronig transformation (using Other Corrections or Interactive Kramers-Kronig in the Process menu), be careful not to bring any data points below zero absorbance. Kramers-Kronig transformation does not work for peaks having negative absorbance values. ▲

6. Click the next baseline point you want to correct.

You can click a point anywhere in the original spectrum; there is no need to correct the baseline from left to right or in any other order.

A line segment is drawn between the two points you have clicked, and the baseline is corrected between those points on the spectrum in the lower pane.



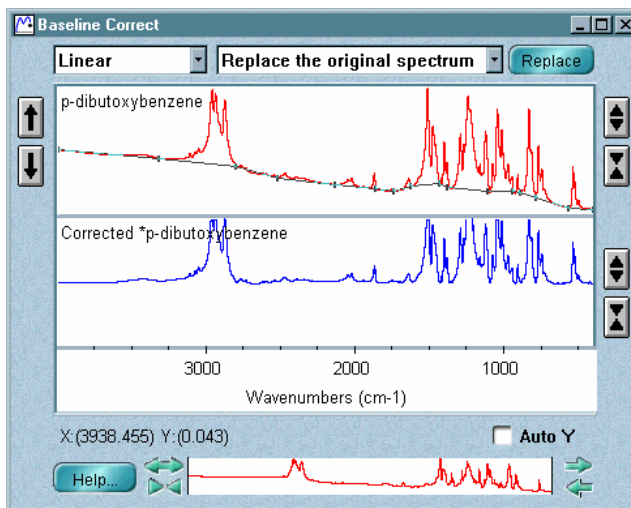
## 7. Click the rest of the baseline points you want to correct.

As you click additional points, a line segment is drawn between adjacent points and the baseline is corrected between the points on the spectrum in the lower pane. Click as few points as necessary to draw a smooth baseline that will straighten pronounced curves or slopes.

You can use the view finder to enlarge a portion of the spectrum to make it easier to click baseline points. The displayed X range of both the original and corrected spectra is affected by the view finder.

To move one of the points you clicked and the line segments that contain the point, drag the point to a new location. To delete a point from the correction, click the point and then press the Delete key. The corrected spectrum is updated automatically.

Here is an example showing a baseline corrected across the entire spectrum:



8. **When you are finished correcting the baseline, you can replace the original spectrum with the corrected version or add the corrected spectrum to a spectral window.**

To do this, select the desired option from the window selection box near the top of the Baseline Correct window and then choose Add or Replace. To close the Baseline Correct window without placing the corrected spectrum into a spectral window, click the Close button.

## Correcting baselines automatically

Automatic Baseline Correct in the Process menu lets you automatically correct the tilted baseline of the selected spectra, with the baseline points selected by the software. See “Why isn’t a baseline always flat and at zero absorbance?” and “What are the benefits of correcting baselines?” earlier in this chapter for more information.

To specify the polynomial order and number of iterations for the correction, set Polynomial Order and Number Of Iterations in the Process options. See “Specifying the order and iterations for automatic baseline correction” in the “Edit” chapter for details.

**Note** If a baseline is not just tilted but also has other undesirable characteristics, correct it using Baseline Correct. See “Correcting a baseline” for more information. ▲

**— How to —>**

Correct baselines automatically

1. **Select the spectra whose baselines you want to correct.**
2. **Select (with the region tool) or display (with the view finder) the spectral region in which you want the baselines corrected.**
3. **Choose Automatic Baseline Correct from the Process menu.**

## Using Advanced ATR Correction

Use Advanced ATR Correction in the Process menu to correct attenuated total reflection (ATR) spectra for the shifting of infrared absorption bands and the effects of variation in depth of penetration.

**Note** If you want to correct an ATR spectrum only for the effects of variation in depth of penetration, use ATR correction, available through Other Corrections in the Process menu. ▲

The biggest overlooked cause of differences between ATR and transmission spectra is the significant shift of intense infrared absorption bands that can occur with the ATR technique. This shift depends on the refractive indices of both the ATR crystal and the sample and is further affected by the angle of incidence of the infrared beam within the crystal. Correcting for band shift lets you achieve better results when you search an ATR spectrum against a library of transmission spectra.

Advanced ATR Correction provides the parameters needed for optimizing the correction of ATR spectra for both the shifting of bands and variation in depth of penetration.

The **Crystal** drop-down list box lets you select the ATR crystal material that was used to collect the spectrum. The following table shows the refractive index of each material at 2000 wavenumbers.

Crystal Material	Refractive Index	Minimum Allowed Angle
Diamond	2.40	38.8
Germanium (Ge)	4.01	22.1
Zinc selenide (ZnSe)	2.43	38.2
Silicon (Si)	3.42	26.1
AMTIR	2.50	37.0
KRS-5	2.38	39.2
Zinc sulfide (ZnS)	2.25	41.9

The **Angle Of Incidence** text box lets you enter the angle of incidence that was used. (See the specifications for the accessory to obtain this value.) The minimum allowed value, shown in the table above, is 0.1 degree greater than the critical angle for the crystal material. The maximum allowed value is 89.9.

The **Number Of Bounces** text box lets you enter the number of internal reflections of the infrared beam that occurred in the ATR crystal.

The **Sample Refractive Index** text box lets you enter the refractive index of the sample. The entered value must be less than the refractive index of the crystal material. The minimum allowed value is 0.01.

See the documentation that came with your ATR accessory for information about the crystal material, angle of incidence and the number of bounces.

When you correct a spectrum using the command, the following information appears in the collection and processing information for the resulting spectrum: the crystal type and its refractive index, the sample refractive index, the angle of incidence, and the number of bounces.

The spectral features listed below cause problems when you use Advanced ATR Correction.

- A negative offset in the baseline.
- A large positive offset in the baseline.
- A tilted baseline.
- Totally absorbing peaks.
- Large positive or negative artifacts in a difference spectrum.

To prepare a spectrum with any of these features for the application of this command, make sure the spectrum is in absorbance or log (1/R) units and that the appropriate baseline correction has been applied.

### ■ *How to* ➔

Use Advanced ATR Correction

#### 1. **Select the spectrum or spectra you want to correct.**

All of the spectra you correct at one time must have been collected using the same crystal type, angle of incidence, number of bounces and sample refractive index. If you want to correct multiple spectra collected under different conditions, correct them one at a time.

#### 2. **Choose Advanced ATR Correction from the Process menu.**

#### 3. **Select the crystal type you used to collect the spectra from the Crystal drop-down list box.**

#### 4. **Type the angle of incidence in the Angle Of Incidence text box.**

#### 5. **Type the number of internal reflections in the Number Of Bounces text box.**

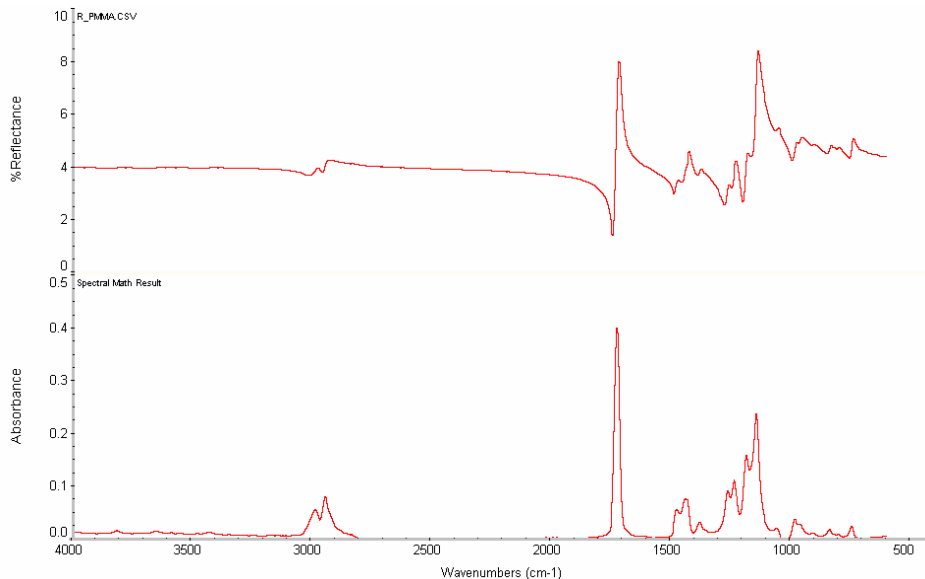
#### 6. **Type the refractive index of the samples in the Sample Refractive Index text box.**

#### 7. **Choose OK.**

## **Performing an interactive Kramers-Kronig transformation**

Use Interactive Kramers-Kronig in the Process menu to convert a specular reflection (SR) spectrum to a transmission-like spectrum that is normalized to 1 absorbance unit (the same result as produced by the Kramers-Kronig option available through Other Corrections in the Process menu) or normalized to a sample thickness of 1 micrometer (the most commonly used output). You can also produce N-index and K-index plots from the data.

The example below shows an SR spectrum and, below it, a resulting transmission spectrum normalized to 1 micrometer and displayed in absorbance units.



SR spectra are the spectra of thick samples with optically smooth surfaces measured using reflection accessories with incident angles less than 30 degrees. An SR spectrum may look like the first derivative of a transmission spectrum, in which an individual peak may have positive and negative peaks relative to the nearby baseline, instead of the usual Gaussian-Lorentzian peaks.

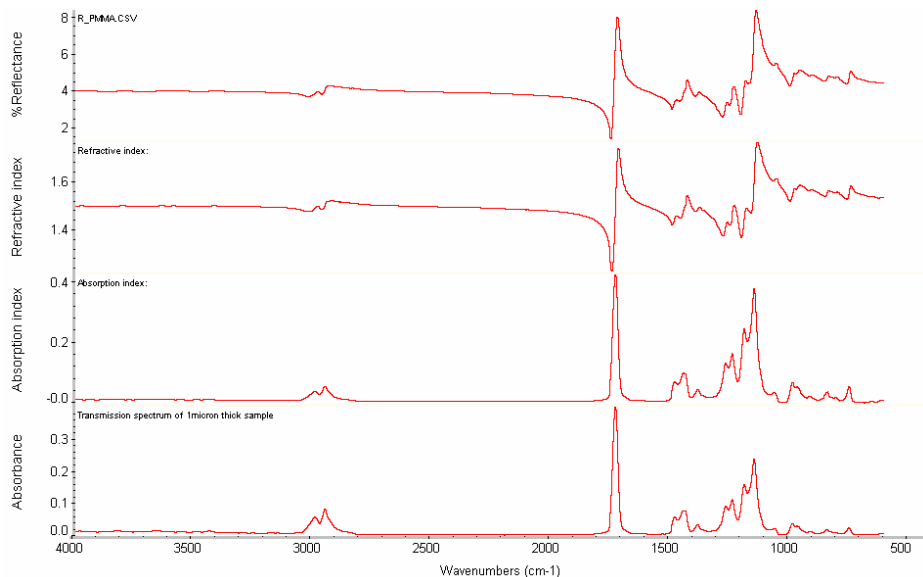
SR spectra are not convenient to use for normal analytical purposes, because their peak positions and intensity ratio, as well as spectral patterns, are different from transmission spectra. They cannot be used for quantitative analyses or as sample spectra in a spectral search.

By applying a mathematical transform called “Kramers-Kronig transformation” to a sample spectrum, you can convert an SR spectrum to an ordinary transmission spectrum. You can then use the converted spectrum for quantitative and qualitative analyses and search this spectrum against the spectra in search libraries.

An N-index plot is a refractive index plot based on the N-index value. A K-index plot is an absorption index plot based on the K-index value. These plots are explained mathematically below.



The following illustration shows an original SR spectrum at the top and, below it, the resulting N-index and K-index plots and transmission spectrum normalized to a sample thickness of 1 micrometer:



A pair of N- and K-indices is called a “complex refractive index” and is sometimes written as

$$\tilde{n} = n + ik \text{ or } \tilde{n} = n - ik, \text{ depending on the author's choice}$$

where  $\tilde{n}$  is the complex refractive index,  $n$  is the refractive index (real part of the complex refractive index),  $i$  is the square root of negative one, and  $k$  is the absorption index (imaginary part of the complex refractive index).

Moreover, in some literatures, the complex refractive index is written as

$$\tilde{n} = n(1 \pm ik)$$

and this pair constitutes the “optical constants” of the sample material. These indices are important for predicting any optical properties such as the ATR spectrum of the sample material with a different ATR crystal at any incident angle for s- and p-polarized light. These indices may be used to calculate SPR and Mie scattering. Also, one can predict ATR, grazing angle reflection-absorption and specular reflection spectra of multilayers on different metal substrates at any incident angle by using complex refractive indices of all the components of multilayers, including substrate and ambient.

**Note** It is documented that Kramers-Kronig transformation gives better results when both the selected beginning and ending frequencies of the spectrum reside in regions where there are no absorption peaks and the baseline is flat. ▲

**Note** Prevent water vapor absorptions by purging the spectrometer. Using the Automatic Atmospheric Suppression option on the Collect tab of the Experiment Setup dialog box may help. You should also remove carbon dioxide by purging. If any carbon dioxide absorptions remain, you can use Straight Line in the Process menu to remove these features. ▲

If you corrected the baseline of a spectrum (using Baseline Correct or Automatic Baseline Correct in the Process menu), try to maintain the baseline level at around 4 %R for ordinary plastic samples. The specular reflectance spectrum of a material with a complex refractive index out of ambient air at near normal incidence is given by

$$R = \frac{(n-1)^2 + k^2}{(n+1)^2 + k^2}$$

For an ordinary plastic, the refractive index,  $n$ , is around 1.5 and the absorption index is zero ( $k = 0$ ), where there is no absorption. Thus,

$$R = (1.5 - 1)^2 / (1.5 + 1)^2 = 4 \%R$$

If the material is not an ordinary plastic, find a refractive index at the sodium D-line from the literature, and estimate the baseline position from the equation shown above at a frequency where there is no absorption.

### ■ **How to** ➡

Perform an interactive Kramers-Kronig transformation

- 1. Select the spectrum you want to transform.**
- 2. Choose Interactive Kramers-Kronig from the Process menu.**

The Interactive Kramers-Kronig dialog box appears.

- 3. Select the types of output to produce.**
- 4. If you selected Absorbance, select the type of normalization to use.**

5. **Select the desired destination window for the new spectrum from the window selection box.**

6. **Choose OK.**

If you selected Add To A New Window and Prompt For New Window Title is turned on in the Window options, a dialog box asks for a title for the new spectral window. Type a title and then choose OK.

The results appear in the specified window.

## Using PAS Linearize

PAS Linearize in the Process menu lets you correct photoacoustic data to enhance the infrared signal at the sample surface or improve quantitative linearity. It requires that interferogram data be available.

The linearization operation uses the method described in R. O. Carter III, *Applied Spectroscopy*, 46, 219 (1992), with the additional operation of shifting the reference interferogram relative to the sample interferogram to make sure that the ZPD points are matched. An application example can be found in Eric. Y. Jiang et al, *Spectroscopy*, 13 (2), 21-40 (1998).

### ■ *How to* ➔

Use PAS Linearize

1. **Obtain a photoacoustic interferogram of glossy carbon black and a photoacoustic interferogram of your sample.**

The two interferograms must have been collected under the same conditions (resolution, optical velocity or phase modulation, etc.). If the carbon black interferogram was not obtained using Collect Background in the Collect menu, save it as a named file.

2. **On the Bench tab of the Experiment Setup dialog box, set Max Range Limit and Min Range Limit to values that are appropriate for the spectra.**

This should be based on the cutoff frequencies of the detector and the spectral range of interest.

### 3. Select the sample interferogram.

If there are multiple sample interferograms, select only one.

### 4. Choose PAS Linearize from the Process menu.

The PAS Linearize dialog box appears.

### 5. Specify the reference spectrum.

If the carbon black interferogram was measured using Collect Background, the Use Current Background option is available. Select it if you want the current background to be used as the reference. Otherwise, select Use Selected File and use the Browse button to locate and select the file containing the glossy carbon black interferogram. You can also type the path to the file in the text box to left of the Browse button.

### 6. Choose OK.

The linearized photoacoustic spectrum of the sample appears.

**Note** This linearized spectrum is also intensity-normalized, so no further normalization against carbon black data is required. ▲

## Using Other Corrections

Use Other Corrections in the Process menu to correct spectra for variations in the depth of penetration or for water or carbon dioxide absorptions or to convert a specular reflection spectrum to a transmission spectrum. When you choose Other Corrections, a dialog box lets you select one of the following correction options.

- Kramers-Kronig
- ATR
- H2O
- CO2
- H2O And CO2

## **Kramers-Kronig transformation**

Kramers-Kronig converts a specular reflection (SR) spectrum to a transmission spectrum displayed in absorbance units and normalized to a maximum value of 1 absorbance unit. SR spectra are the spectra of thick samples with optically smooth surfaces measured using reflection accessories with incident angles less than 30 degrees. An SR spectrum may look like the first derivative of a transmission spectrum, in which an individual peak may have positive and negative peaks relative to the nearby baseline, instead of the usual Gaussian-Lorentzian peaks.

SR spectra are not convenient to use for normal analytical purposes, because their peak positions and intensity ratio, as well as spectral patterns, are different from transmission spectra. They cannot be used for quantitative analyses or as sample spectra in a spectral search.

By applying a mathematical transform called "Kramers-Kronig transformation" to a sample spectrum, you can convert an SR spectrum to an ordinary transmission spectrum. Then you can use the converted spectrum for quantitative and qualitative analyses and search this spectrum against the spectra in search libraries.

Due to the nature of Kramers-Kronig transformation, it gives better results when both the beginning and ending frequencies of the spectrum reside in flat spectral regions.

For best results, remove water vapor and carbon dioxide absorptions from your spectra by purging the spectrometer. Using the Automatic Atmospheric Suppression option on the Collect tab of the Experiment Setup dialog box may help. You can also use Straight Line in the Process menu to remove these features.

You can also use Interactive Kramers-Kronig in the Process menu to perform a Kramers-Kronig transformation. It give you the choice of normalizing the spectrum to 1 micrometer sample thickness or 1 absorbance unit and also lets you produce refractive index and absorption index plots. See "Performing an interactive Kramers-Kronig transformation" for more information.

## **ATR correction**

Use ATR to correct spectra collected using the attenuated total reflection (ATR) technique for the effects of variation in the depth of penetration.

**Note** Use Advanced ATR Correction in the Process menu if you want to correct ATR spectra for both the effects of variation in the depth of penetration and the shifting of infrared absorption bands that occurs with the ATR technique. See “Using Advanced ATR Correction” for details. ▲

In the ATR technique, the depth of penetration (that is, the effective pathlength) of the infrared beam varies as a function of the wavelength of light: The longer wavelengths (lower frequencies) penetrate the sample more deeply than do the shorter wavelengths (higher frequencies). As a result, the peaks at lower frequencies are much stronger than those at higher frequencies. This skewing of peak intensities causes problems when you search a sample spectrum against a library of normalized spectra collected using standard transmission techniques, since the peaks have a different appearance.

Before searching an ATR spectrum against a library of normalized transmission spectra or a library of corrected ATR spectra, correct the spectrum. (If you search a library of uncorrected ATR spectra, do not correct the sample spectrum.)

ATR correction multiplies the sample spectrum by a wavelength-dependent factor to adjust the relative peak intensities. The resulting spectrum has peaks more like those in a spectrum collected by transmission and can be visually compared with transmission spectra or searched against a library of transmission spectra.

### **Water correction**

Use H<sub>2</sub>O to correct a spectrum for the effects of water. This requires the use of a water reference spectrum. See “Specifying water and carbon dioxide reference spectra” in the “Edit” chapter for a procedure for collecting one.

### **Carbon dioxide correction**

Use CO<sub>2</sub> to correct a spectrum for the effects of carbon dioxide. This requires the use of a carbon dioxide reference spectrum. See “Specifying water and carbon dioxide reference spectra” in the “Edit” chapter for a procedure for collecting one.

## Water and carbon dioxide correction

Use H<sub>2</sub>O And CO<sub>2</sub> to correct a spectrum for the effects of water and carbon dioxide. This requires the use of a water and carbon dioxide reference spectrum. See “Specifying water and carbon dioxide reference spectra” in the “Edit” chapter for a procedure for collecting one.

In a typical FT-IR experiment the sample spectrum is ratioed against a background spectrum that contains all of the spectral characteristics of the instrument. These characteristics include absorptions due to any atmospheric water vapor and carbon dioxide inside the spectrometer. Ratioing ensures that the sample spectrum contains information that is characteristic only of the sample.

Since you collect the sample and background spectra separately, the water and carbon dioxide absorptions may not be exactly the same in both spectra. This can result in small positive (or negative) peaks in the water (3,800 and 1,600 wavenumbers) and carbon dioxide (2,350 and 668 wavenumbers) regions of the ratioed sample spectrum. These residual peaks will cause problems when you search the spectrum against a library.

If you use Other Corrections, the water and carbon dioxide correction involves subtracting a reference spectrum of pure water and carbon dioxide (or of just one) from the sample spectrum to remove the correct amount of each component. Since a pure reference is used, only the water and carbon dioxide absorptions are affected.

If you use Automatic Atmospheric Suppression on the Collect tab of the Experiment Setup dialog box, the effects of water vapor and carbon dioxide are automatically suppressed through the use of a quantitative model. We recommend using this feature instead of the water and carbon dioxide corrections available through Correction on the Collect tab of the Experiment Setup dialog box or Other Corrections in the Process menu, unless you find that the humidity in your facility is too high for it to work effectively.

### ■ *How to* ➔

Process spectra using Other Corrections

#### 1. Select the spectra.

If you are performing a Kramers-Kronig transformation, display the spectral region that you want transformed. Only this region will be included in the new spectra.

**2. Choose Other Corrections from the Process menu.**

The Other Corrections dialog box appears.

**3. Select an option from the drop-down list box.**

**4. Choose OK.**

## Blanking a spectral region

Use Blank in the Process menu to delete the data points in the selected spectral region of the selected spectra (or in the displayed region if no region is selected).

**Note** You can also blank spectral regions during data collection by using Automatic Blanking Of Regions on the Advanced tab of the Experiment Setup dialog box. See “Blanking spectral regions during data collection” in the “Collect” chapter for details. ▲

## When to blank a spectral region

Blanking a spectral region can improve your data in the following situations:

- A spectrum contains totally absorbing peaks (having an absorbance value greater than 3) because the sample is too thick. The random noise at the top of these peaks will cause poor results when you search the spectrum against a library or quantify or subtract the spectrum.
- A spectrum includes the region below the cutoff of an MCT detector (approximately 700 wavenumbers) or the cutoff of an ATR crystal. (Normally you should adjust the saved spectral range before data collection to eliminate these regions.) These regions contain only noise since there is no spectral information present. If you don't eliminate these regions, they will interfere with library searches and spectral processing.
- A spectrum contains derivative-shaped artifacts following subtraction of a reference spectrum. These artifacts can occur when molecular interactions cause peaks to shift relative to the peaks in the reference spectrum. The artifacts can cause problems when you search the subtraction result against a spectral library.



- You want to display a spectrum full scale to better view its peaks but a totally absorbing band interferes.
- A spectrum has a region you want ignored when searching a spectral library.

**Note** Immediately after you blank a spectral region, you can restore it by using Undo in the Edit menu. If you save a spectrum after blanking one of its regions, you can restore the region only by using Reprocess in the Process menu. ▲

## The difference between Blank and Straight Line

Straight Line in the Process menu draws a straight line between the points adjacent to the edges of the selected region, while Blank simply deletes the points in the selected region. The change made to a spectrum by replacing a region with a straight line may not be apparent to someone who examines the spectrum. Blanking the region, on the other hand, makes it apparent that the original data have been removed from that region.

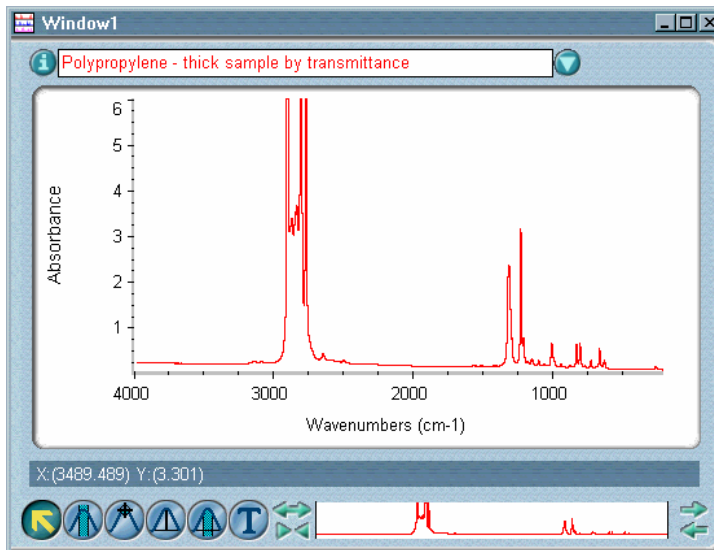
Also, if you replace with a straight line a region that contains peaks and then search the spectrum against a library, any library spectra with peaks in that region will be considered to be very different from the sample spectrum. This is unlike searching a library to identify a spectrum in which the region was blanked. In that case, the region is simply ignored.

See “Replacing a spectral region with a straight line” for complete information on the Straight Line command.

## — *How to* → Blank a spectral region

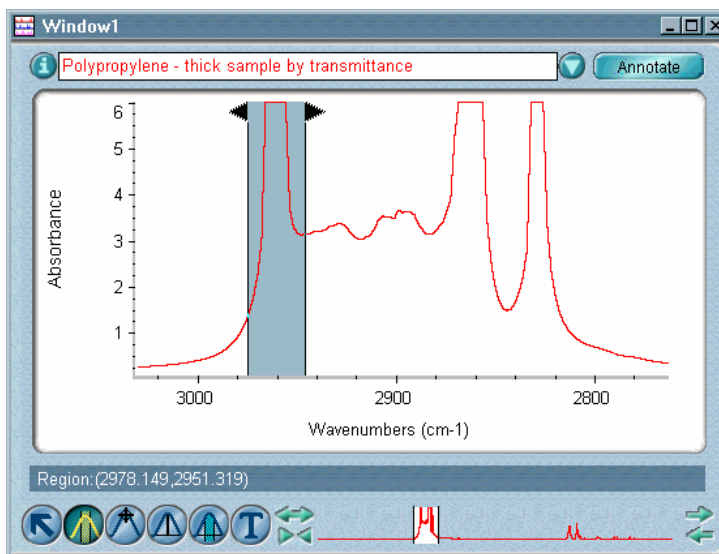
### 1. Select the spectra that contain the spectral region.

The spectra can be in any units. The following example shows a spectrum with totally absorbing peaks between 3000 and 2800  $\text{cm}^{-1}$ .



### 2. Use the region tool to select the spectral region.

(If you do not select a region, the entire displayed region will be blanked.)  
To make it easier to select the region, you can first use the view finder, selection tool or Roll/Zoom window to expand the display.



### 3. Choose Blank from the Process menu.

The region you selected is erased. Any annotation associated with the blanked region is also deleted.

## Replacing a spectral region with a straight line

Straight Line in the Process menu lets you replace the selected region of the selected spectra (or the displayed region if no region is selected) with data points that form a straight line. Use Straight Line to remove unwanted spectral features such as totally absorbing bands in order to improve the appearance of a spectrum.

See “The difference between Blank and Straight Line” for more information.

**Note** Don't use Straight Line to replace bands that contain important spectral information. ▲

**Note** Immediately after you replace a spectral region with a straight line, you can restore it by using Undo in the Edit menu. If you save a spectrum after replacing one of its regions, you can restore the region only by using Reprocess in the Process menu. ▲

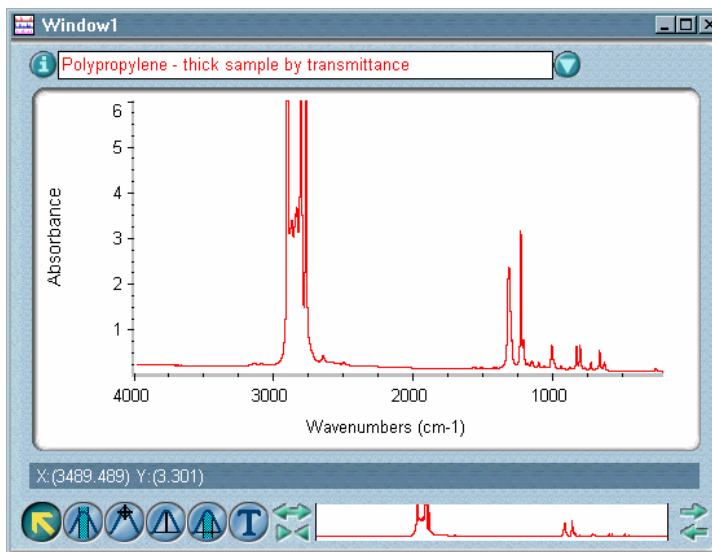
### — How to ➡

Replace a spectral region with a straight line

#### 1. Select the spectra that contain the spectral region.

The spectra can be in any units.

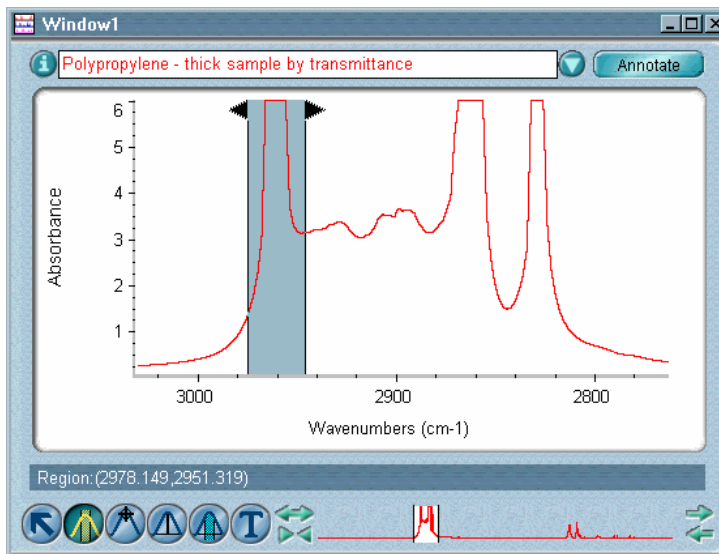
The following example shows a spectrum with totally absorbing peaks between 3000 and 2800 wavenumbers.



## 2. Use the region tool to select the spectral region.

If you do not select a region, the entire displayed region will be replaced with a straight line.

To make it easier to select the region, you can first use the view finder, selection tool or Roll/Zoom window to expand the display.



### 3. Choose Straight Line from the Process menu.

A straight line is drawn between the two data points at the limits of the selected spectral region.

## Subtracting spectra

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.

### How does spectral subtraction work?

When you use Subtract to subtract one spectrum from another, the software calculates data point by data point the difference between the two.

According to the Beer-Lambert law, the spectrum of a sample that is a mixture of two materials (components A and B) is the sum of the spectra of the two materials. If you subtract the spectrum of one pure component (for example, B) from the mixture spectrum, the result is a spectrum of the other pure component (A). This can be expressed by the equation  $(A + B) - B = A$ .

In most cases spectra are not subtracted on a one-to-one basis, since the components do not have the same concentration and so their intensities do not match. For example, a mixture may be 20% component A and 80% component B, or it might be 90% A and 10% B. If you first scale a reference spectrum of component B so that its intensities match those in the mixture spectrum, you can then cleanly subtract out the peaks due to component B, leaving only peaks due to component A.

Consider this example: You have used a fixed-path cell to collect a sample spectrum of a 10% solution of a compound in an organic solvent. You decide to collect a reference spectrum of the pure solvent using the same cell so that you can subtract the reference spectrum from the sample spectrum to produce a spectrum of the compound alone. If you subtract the spectra without scaling, the result will exhibit overcompensation for the solvent peaks (giving negative peaks) since the “reference” is 100% solvent while the “sample” is only 90% solvent. The answer is to first scale the reference spectrum to 90% so that the subtraction result will be “clean.” The scaling factor is called the “subtraction factor.”

Algebraically, the subtraction works like this:

$$\text{Sample} - \text{Reference} * \text{Factor} = \text{Result}$$

You determine the subtraction factor interactively by watching the changes in the common peaks as you change the factor. If the common peaks in the result spectrum are becoming smaller, you know you are changing the factor in the right direction. The optimum factor is one which produces nulled (or zeroed) common peaks in the subtraction result. If you use the correct factor, the peaks present in the result will be due solely to the sample material of interest.

### **When to use spectral subtraction**

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

- If you collect a spectrum of a sample that is dissolved in a solvent, the spectrum will contain peaks due to the solvent. By subtracting a spectrum of the pure solvent from the sample spectrum, you can eliminate the solvent peaks and produce a “clean” spectrum of the sample material.
- When you collect a spectrum of a sample that is a mixture of two or more components, the spectrum is, theoretically, the sum of the spectra of all the components. By subtracting a spectrum of a pure component from the sample spectrum, you can produce a simpler mixture spectrum. This is a means of “separating” components of a mixture without having to do it physically.
- If you collect a spectrum of a sample that contains an unknown contaminant, the spectrum will contain peaks due to the contaminant. By subtracting a spectrum of uncontaminated sample material from the first spectrum, you can produce a residual spectrum of the contaminant. You can then search that spectrum against a library to identify the contaminant.
- If you collect a series of spectra to monitor a kinetic process such as a chemical reaction or curing, the spectra will reflect the chemical changes that occur. By subtracting a “time zero” spectrum (collected before the start of the process) from the subsequent spectra, you can produce spectra that will help you determine what has changed.

- Subtraction is the most critical form of spectral comparison. If you collect spectra to monitor the quality of a material being produced, you can more easily detect changes from one batch to the next by subtracting one sample spectrum from the next (or vice versa) than by just comparing the spectra visually.
- Subtracting spectra is useful when you want to make simple comparisons in applications like these:

inspection of incoming raw materials

comparison of batches or samples

evaluation of organic reactions

failure analysis

contaminant analysis

analysis of coatings

comparison of an unknown with library spectra

spectral search of a mixture spectrum

### ■ *How to* ➡

Subtract a spectrum from another spectrum

- 1. Select the two spectra on which you want to perform the subtraction.**

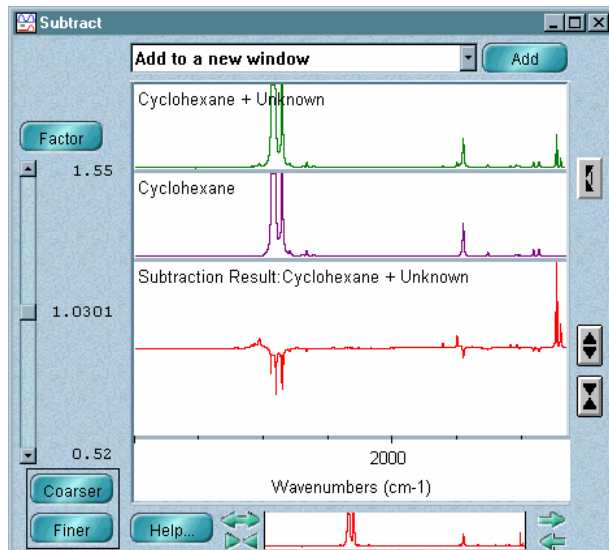
Remember to hold down the Control key when selecting the second spectrum.

First select the spectrum from which you want to subtract spectral features; this is the sample spectrum. Then select the spectrum with the features you want to subtract from the sample spectrum; we will call this the reference spectrum.

## 2. Choose Subtract from the Process menu.

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

The Subtract window appears with the sample spectrum displayed in the top pane and the reference spectrum below it.



**Note** If the spectra do not have the same resolution, the spectrum with the higher resolution will be temporarily deresolved to match the resolution of the other spectrum. The subtraction operation will take longer in this case. ▲

The spectral region displayed in the Subtract window is the same region that was displayed when you chose Subtract. To display a different region of all the spectra, use the view finder.

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.

To expand or contract the Y-axis of the difference spectrum, click the buttons to the right of the bottom pane. Expanding the spectrum helps you see small features.



Each time you click the Expand button, the scale of the Y-axis doubles.



Each time you click the Contract button, the scale of the Y-axis is reduced by one-half.





If you want to reverse the order of subtraction, click the double-arrow to the right of the spectra. The order of the spectra is reversed and the new difference spectrum is displayed in the bottom pane.

### 3. **If you are not satisfied with the result, try changing the subtraction factor.**

The current factor was calculated using the spectral data displayed when you chose Subtract. If you change the factor, the new difference spectrum will be automatically displayed in the bottom pane. There are two ways to change the factor: by using the scroll bar or by typing a new value.

- To change the factor using the scroll bar, drag the scroll box or click the scroll arrows. The current upper and lower limits of the scroll bar range appear near the upper and lower scroll arrows, respectively.

The factor is displayed between the limits. To increase or decrease the range of the scroll bar, choose Coarser or Finer. Each time you choose Coarser, the range is doubled; changes you subsequently make to the factor by clicking the scroll arrows or dragging the scroll box will be twice as large. Each time you choose Finer, the range is reduced by one-half and changes you make to the factor by clicking the scroll arrows or dragging the scroll box will be half as large. Choosing Coarser or Finer does not change the current value of the subtraction factor displayed next to the scroll bar; only the number of decimal places in the factor setting may be affected.

- To change the factor by typing a new value, choose Factor. In the dialog box that appears type a new factor in the text box and then choose OK, or choose Cancel if you don't want to change the factor.

### 4. **When you are satisfied with the difference spectrum, you can replace the sample spectrum with it or add it to a spectral window.**

To do this, select the desired option from the window selection box near the top of the Subtract window and then choose Add or Replace. The title of the spectrum will be "Subtraction Result."

To close the Subtract window without placing the difference spectrum into a spectral window, click its Close button.

## Subtracting a component or contaminant from a mixture spectrum

In addition to the standard Subtract command, OMNIC includes the Automatic Region Subtract command in the Process menu to let you quickly subtract from a mixture or sample spectrum the spectral data due to a particular component or contaminant. By selecting the region of a reference spectrum that contains the undesirable peaks, you allow the software to automatically determine the subtraction factor that will best eliminate those peaks in the mixture or sample spectrum when the spectra are subtracted.

This feature is particularly useful for isolating contaminants, verifying mixture components, and obtaining pure component spectra from microscope-mapping spectra of very thin layers of a sample.

### — *How to* ➔

Subtract a component or contaminant from a mixture spectrum

- 1. Select the spectrum and the reference spectrum that contains the component peaks.**

The order of selection does not matter. Remember to hold down the Control key when selecting the second spectrum.

- 2. Use the region tool to select the spectral region that contains the component peaks.**

- 3. Choose Automatic Region Subtract from the Process menu.**

The result spectrum appears in the spectral window.

#### **Note**

The order of subtraction is automatically determined based on the presence of both common and unshared peaks. ▲

## Performing a Fourier self-deconvolution

Use Fourier Self-Deconvolution in the Process menu to reveal overlapping spectral features that cannot be resolved by collecting data at a higher resolution setting.

**Note** Since the resulting bands are not “real,” you should state that this function was used if you include the spectrum in a report or compare it with other spectra. ▲

By setting Bandwidth and Enhancement, you control the Fourier self-deconvolution (FSD) process to optimize the result. Bandwidth is an estimate of the widths of the overlapped bands. Enhancement is a measure of the degree to which features are revealed. It determines the “strength” of the resolving power applied to the data.

■ *How to* ➡ Perform a Fourier self-deconvolution

**1. Select the spectrum on which you want to perform an FSD.**

**Note** We recommend that the spectrum be in absorbance units. If necessary, use Absorbance in the Process menu to convert it before performing the FSD. ▲

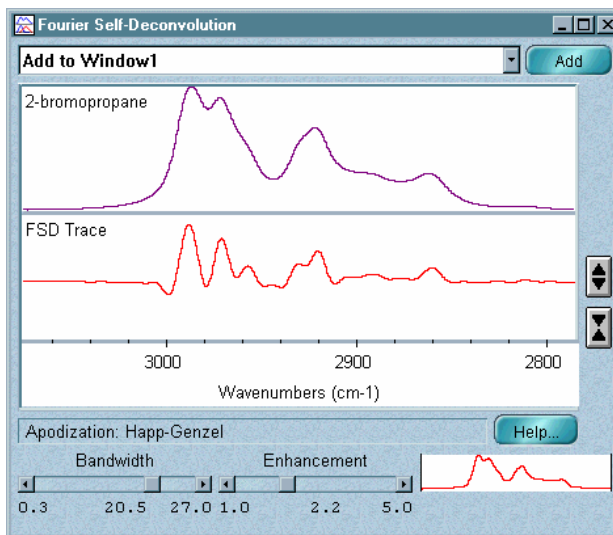
**2. Use the region tool to select the region that contains the features you want to reveal.**

You will be able to display a smaller portion of the spectral region during the operation, but you will not be able to display a larger region.

**3. Choose Fourier Self-Deconvolution from the Process menu.**

The Fourier Self-Deconvolution window shows the original spectrum at the top and the result spectrum below it. The apodization type used when the original spectrum was collected is shown below the result spectrum.

Here is an example:



To display a smaller portion of the spectral region to see the peaks better, use the view finder. The displayed X range of both spectra will be affected.

To expand or contract the Y-axis of the result spectrum, click the buttons to the right of the bottom pane.



Each time you click the Expand button, the scale of the Y-axis doubles.



Each time you click the Contract button, the scale is reduced by one-half.

#### 4. If you are not satisfied with the result, you can change the settings of Bandwidth and Enhancement.

When you change a setting, the new result appears automatically. To change the Bandwidth or Enhancement settings, use the appropriate scroll bar. The current setting is shown below the scroll bar.

**Note** If negative peaks appear in the result, it means they have been “over-resolved.” You can adjust the bandwidth and enhancement to eliminate this problem. ▲

5. **When you are satisfied with the result spectrum, you can replace the original spectrum with it or add it to a spectral window.**

To do this, select the desired option from the window selection box near the top of the FSD window and then choose Add or Replace.

To close the FSD window without placing the result spectrum into a spectral window, click its Close button.

## Smoothing spectra

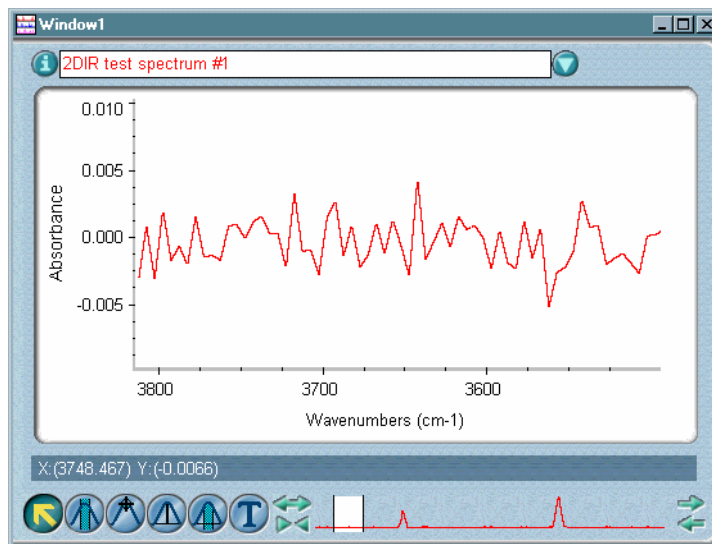
Use Smooth in the Process menu to improve the appearance of the selected spectra by preferentially smoothing the high-frequency component of the spectral data. Smoothing is useful for improving the appearance of peaks obscured by noise. Smooth uses the Savitzky-Golay algorithm.

**Note** If you want to smooth spectra manually by specifying the degree of smoothing (setting the number of points), use Smooth. To smooth spectra automatically, use Automatic Smooth. An automatic smooth often gives a satisfactory result and is faster than a manual smooth. See “Smoothing a spectrum automatically” for more information. ▲

### Setting the number of points

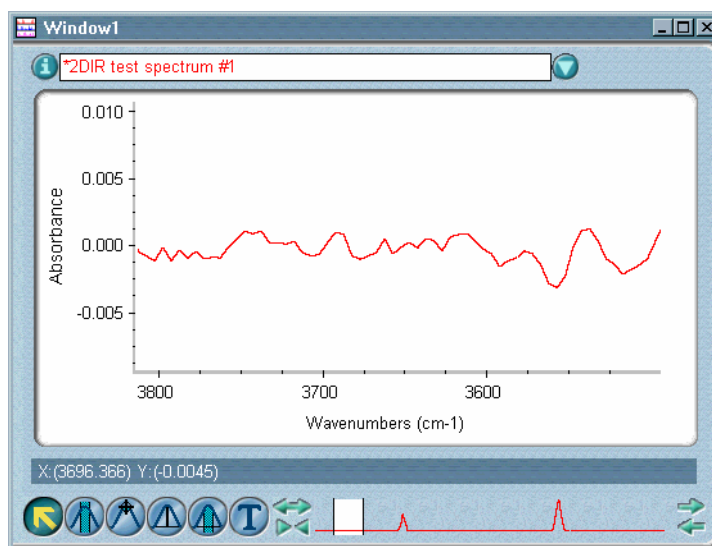
The degree to which a spectrum is smoothed depends on the number of points used in the smoothing process. You can set the number of points to any odd number from 5 to 25. A larger number of points results in a greater degree of smoothing. You should normally smooth using the minimum number of points that produce the desired result.

The following example shows a region of a spectrum.



Here is the same region after being smoothed using 7 smooth points:

Notice that the peaks are not as sharp as they were before smoothing.



**Note** If you smooth more than one spectrum at the same time, all the spectra must have the same data point spacing. ▲

For moderate smoothing of a spectrum at 4- or 8-wavenumber resolution, start with 5, 7 or 9 points. Compare the sharpest bands in the original spectrum with the same bands in the smoothed spectrum to determine whether the resolution was degraded significantly. If the resolution was not significantly degraded, increase the number of points and smooth again if needed.

## ■ *How to* ➡ Smooth spectra

1. **Select the spectra.**
2. **Choose Smooth from the Process menu.**

The Smooth dialog box appears.

3. **Select the desired number of smooth points from the drop-down list box.**

The value to the right of the number of points represents the frequency range that is considered when smoothing a point in a spectrum. The value is the product of the number of smooth points and the data spacing of the spectrum.

4. **Choose OK.**

## Smoothing spectra automatically

Use Automatic Smooth in the Process menu to improve the appearance of the selected spectra by automatically smoothing the high-frequency component of the sample data. Smoothing is useful for improving the appearance of peaks obscured by noise.

**Note** If you want to smooth spectra manually by specifying the degree of smoothing (setting the number of points), use Smooth. To smooth spectra automatically, use Automatic Smooth. An automatic smooth often gives a satisfactory result and is faster than a manual smooth. See “Smoothing spectra” for more information. ▲

## ■ *How to* ➡ Smooth spectra automatically

1. **Select the spectra.**
2. **Choose Automatic Smooth from the Process menu.**

## Changing the data spacing of spectra

Use Change Data Spacing in the Process menu to change the spacing of the data points in the selected spectra to a value you select.

**Note** If a spectral region is selected, only that region is included in the resultant spectra. ▲

Data spacing is the number of wavenumbers between data points in a spectrum. It is determined by the resolution and zero filling settings used when you collect the spectrum.

If you use this command to change the data spacing of a spectrum to a higher value, the software deresolves the spectrum. If you change the data spacing of a spectrum to a lower value, the software zero fills the data; that is, it adds interpolated data points between the existing data points.

You can best compare two spectra if they have the same data spacing. If the spectra were collected using different spacings, you can use this command to change the data spacing of one spectrum to match the other.

For example, if you search a deresolved library—with a data spacing of  $8\text{ cm}^{-1}$ —to identify an unknown spectrum with a data spacing of  $2\text{ cm}^{-1}$ , the software will deresolve the unknown and then do the search. However, your visual comparison of the unknown spectrum and the best matches from the library will be hindered because of the difference in data spacing. By changing the data spacing of the unknown spectrum to  $8\text{ cm}^{-1}$ , you can make a better visual comparison.

In quantitative analysis the data spacing of the sample spectrum must match the standard spectra used to develop the method. You can use this command to change the data spacing of a sample spectrum to match the standards before the analysis.

To subtract spectra of different resolutions, change the data spacing of the lower resolution spectrum to match the higher resolution spectrum. This adds interpolated data points between existing points in the lower resolution spectrum (zero fills), so the data points of the spectra line up when you perform the subtraction.



**— How to ➡**

Change the data spacing of spectra

**1. Select the spectra.**

If you want the resultant spectra to include only a particular spectral region, use the region tool to select that region.

**2. Choose Change Data Spacing from the Process menu.**

The Change Data Spacing dialog box appears.

**3. Select a data spacing setting from the drop-down list box.****4. Choose OK.**

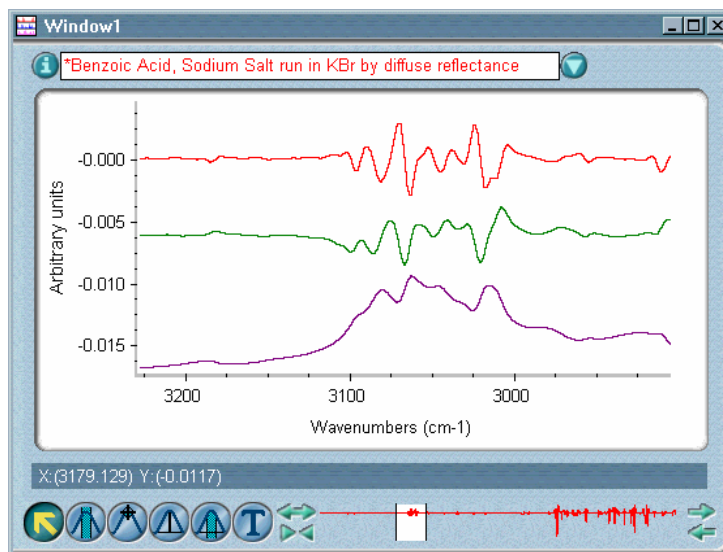
## Converting spectra to their first or second derivatives

Use Derivative in the Process menu to convert the selected spectra to their first or second derivatives. The original spectra can be in any units when you use Derivative; however, the derivative operation is usually applied to absorbance, Kubelka-Munk or photoacoustic spectra.

The **first derivative** is useful for revealing peaks that appear as shoulders in the original spectra. It shows the rate of change across the entire spectrum. This means that in the first derivative, shoulders become narrower and thus are easier to see. It is important to remember that the maximum and minimum points in the first derivative curve are the points of maximum rate of change and not the maximum and minimum points of the original peaks. The maximum and minimum points of the original peaks have a Y value of zero in the first derivative.

Use the **second derivative** to find the exact location (center) of shoulders in the original spectra. It shows the change in the rate of change across the spectrum. This curve is more complex than the first derivative, with significantly narrower bands. The second derivative is useful for finding exact peak locations since peaks in the second derivative appear at the same locations as peaks in the original spectrum. The second derivative has more baseline noise than the first derivative. For each derivative operation you perform, the noise level increases slightly, the signal strength decreases dramatically and the signal-to-noise ratio decreases.

The following example shows a spectrum with the first derivative above it and the second derivative at the top.



You can specify that the conversion be done using no filter, using the Savitzky-Golay derivative filter, or using the Norris derivative filter:

- Select the **First Difference Derivative** option if you do not want to use a filter.
- The **Savitzky-Golay Derivative** option is useful for improving the appearance of peaks that are obscured by noise. It uses the specified number of data points and polynomial order to determine the degree of smoothing for the conversion.

You can set the number of data points to any odd number from 3 to 51. A larger number results in a greater degree of smoothing. You should normally smooth using the minimum number of data points that produce the desired result. Typically a setting of 7 is used for average smoothing.

For moderate smoothing of a spectrum at 4- or 8-wavenumber resolution, start with a setting of 5, 7 or 9. Compare the sharpest bands in the original spectrum with the same bands in the smoothed spectrum to determine whether the resolution was degraded significantly. If it was not, increase the number of data points and smooth again if needed.

You can set the polynomial order to any number from 1 to 6 (the default value is 3). A higher polynomial order results in less smoothing; lower orders cause more smoothing. Typically a setting of 3 (for cubic polynomial) is used for average smoothing.

**Note** The setting of Polynomial Order must be smaller than the setting of Points. If the polynomial order is greater than the number of data points for smoothing, any additional polynomial coefficients are automatically set to zero. ▲

**Notice** The Savitzky-Golay algorithm smooths all peaks. Smoothing degrades the effective spectral resolution of the data and can remove ("smooth out") small spectral features, including sample peaks, especially those in mid-IR spectra. ▲

- The **Norris Derivative** option is typically applied to near-IR spectra. It is often used to enhance a sharp band that is overlapped by another broad band. It is also useful for improving the appearance of peaks that are obscured by noise.

The Norris Derivative option uses the segment length and gap between segments to determine the degree of smoothing. We define the gap between segments as the distance, in number of data points, between two consecutive segments.

You can set the segment length to any odd number from 1 to 51 (the default value is 5). Increasing the length results in greater smoothing, since the length determines how many points are averaged.

You can set the size of the gap to any number from 1 to 20 (the default value is 5). Increasing the gap may enhance a sharp band that is overlapped by another broad band. A larger gap will also produce larger differences for broad peaks and tend to lower the resolution of the spectrum.

■ **How to** ➡ Convert spectra to their first or second derivatives

1. **Select the spectra.**
2. **Choose Derivative from the Process menu.**

The Derivative dialog box appears.

**3. Select a derivative order from the Derivative drop-down list box.**

**4. Select the filter option you want to use.**

If you selected First Difference Derivative, go to step 6. If you selected another option, continue with the next step.

**5. Set the parameters for the selected filter option.**

- If you selected Savitzky-Golay Derivative, set Points to an odd number from 3 to 51; a higher setting results in greater smoothing. Set Polynomial Order to any number from 1 to 6; a higher setting results in less smoothing.
- If you selected Norris Derivative, set Segment Length to an odd number from 1 to 51; a higher setting results in greater smoothing. Set Gap Between Segments to any number from 1 to 20; a higher value tends to lower the resolution of the spectrum.

**6. Choose OK.**

## Multiplying a spectrum by a number

Use Multiply in the Process menu to multiply each data point in a spectrum by a number of your choice. This is useful when you want to scale a spectrum so that data of very different intensities can be compared. By making the intensity of a peak in one spectrum match that of the same peak in another spectrum, you can see how the relative intensities of the other peaks compare.

### — *How to* ➔

Multiply a spectrum by a number

**1. Select the spectrum that you want to multiply.**

**2. Choose Multiply from the Process menu.**

The Multiply dialog box requests the number to be used.

3. **Type a number in the text box.**

4. **Choose OK.**

The spectrum is multiplied by the number you entered and displayed as a new spectrum in the same spectral window.

## Adding spectra

Use Add in the Process menu to add together two spectra that have the same Y-axis unit. When spectra are added, each data point of one spectrum is added to the corresponding data point of the other spectrum.

If only one of the spectra contains data points in a spectral region, the Y value of the other spectrum is considered to be zero in that region when the spectra are added.

### — *How to* ➔

Add a spectrum to another spectrum

1. **Select the two spectra you want to add together.**

(Hold down the Control key when you select the second spectrum.)  
The spectra must be in the same spectral window. If they are not, first copy and paste one of the spectra into the window that contains the other.

2. **Choose Add from the Process menu.**

The spectra are added together and the result is displayed in the window that contains the original spectra.

## Performing arithmetic operations on spectra

Use Spectral Math in the Process menu to perform arithmetic operations on one or two selected spectra. You specify the operations to perform by typing or selecting 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 lets you type the desired operations in the Operation text box. You can also select one of the operations provided in the Operation drop-down list box.

For example, if you are subtracting a single-component reference spectrum from a spectrum of a mixture of two components, select (or type) the operation

$$A - k*B$$

where A is the mixture spectrum, k is the subtraction factor and B is the single-component spectrum. The result of the operation is a spectrum of the other component.

The following table explains the symbols that you can use and gives some examples.

Symbol	Meaning	Examples
A	Spectrum A.	
B	Spectrum B, if used.	
+	Add.	A+1: 1 added to spectrum A. A+B: Sum of Spectrum A and Spectrum B.
-	Subtract.	-A: Spectrum A multiplied by -1. A-1: 1 subtracted from Spectrum A. A-B: Spectrum B subtracted from Spectrum A.
*	Multiply.	A*1.25: Spectrum A multiplied by 1.25. A*B: Spectrum A multiplied by Spectrum B.
/	Divide.	A/2: Spectrum A divided by 2. A/B: Spectrum A divided by Spectrum B. 1/A: Reciprocal of Spectrum A. (A+B)/2: Average of Spectrum A and Spectrum B.

Symbol	Meaning	Examples
k	Factor set with Factor button or scroll bar.	k*A: Spectrum A multiplied by k.
D	First derivative.	DA: First derivative of Spectrum A. DA+DB: Sum of first derivatives of Spectrum A and Spectrum B.
DD	Second derivative.	DDA: Second derivative of Spectrum A.
log	Logarithm (base 10).	logA: Logarithm of Spectrum A.
exp	Exponent of 10.	exp(-3): 10 raised to negative third power. expA: 10 raised to power of Spectrum A.
sqrt	Square root.	sqrtA: Square root of Spectrum A. sqrt(A*B): Square root of product of Spectrum A and Spectrum B.
100 (or other number)	Fixed Y value.	100: Flat line at Y = 100.

Type the desired operations just as you would any mathematical equation, except do not include an equals sign (=) at the end. The software uses the standard order of priority when performing the operations; that is, multiplication and division before addition or subtraction, and operations to the left before those to the right when they have the same priority. Use parentheses to change the order just as in a normal mathematical equation. Special operations such as D (first derivative), DD (second derivative), log (logarithm), exp (exponent) and sqrt (square root) are performed before other operations unless the other operations are enclosed in parentheses.

Here is an example showing several different operations:

$$(A+B)/2-\log(A/100)+k*A*DB$$

Your operations will probably be much simpler.

**Note** If you want to add two spectra or subtract one from another, the spectra must have the same Y-axis unit. If necessary, use a command in the Process menu to convert one of the spectra to the Y-axis format of the other before choosing Spectral Math. ▲

**Note** If you combine (by adding) two spectra with different spectral ranges, the resulting spectrum will contain only the spectral region that is common to both. This is unlike using the Add command, which results in a spectrum whose range is the union of the ranges of the two original spectra. ▲

➡ **How to** ➡ Perform arithmetic operations on spectra

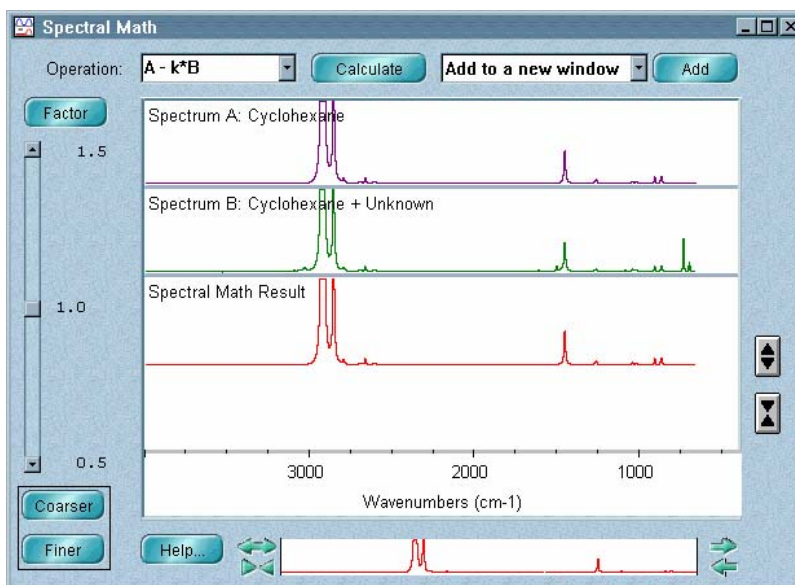
### 1. Select the spectra on which you want to perform the arithmetic.

You can select one or two spectra. Remember to hold down the Control key when selecting a second spectrum.

The spectra must be in the same spectral window. If they are not, first copy and paste one of the spectra into the window that contains the other.

### 2. Choose Spectral Math from the Process menu.

The Spectral Math window appears with the selected spectrum or spectra displayed in the upper pane or panes. Here is an example:





The title of each spectrum appears in its pane. The spectrum you selected first appears in the top pane. When you specify the operation, this spectrum is represented by the constant A. If you selected two spectra, the second spectrum is represented by the constant B.

**Note** If the spectra don't have the same resolution, the spectrum with the higher resolution will be temporarily deresolved to match the resolution of the other spectrum. ▲

The spectral region displayed in the window is the same region that was displayed when you chose Spectral Math. To display a different region of all the spectra, use the view finder.

### 3. **Select an operation from the Operation drop-down list box or type an operation in the Operation text box.**

If you include the factor k, you can change its value in two ways: by using the scroll bar to the left of the subtraction result or by typing a new value.

- To change the factor using the scroll bar, drag the scroll box or click the scroll arrows. The current upper and lower limits of the scroll bar range appear near the upper and lower scroll arrows, respectively.

The current factor is displayed between the limits. You can increase or decrease the range of the scroll bar by choosing Coarser or Finer.

Each time you choose Coarser, the range is doubled. As a consequence, changes you subsequently make to the factor by clicking the scroll arrows or dragging the scroll box will be twice as large. Each time you choose Finer, the range is reduced by one-half and changes you make to the factor by clicking the scroll arrows or dragging the scroll box will be half as large. Choosing Coarser or Finer does not change the current value of the subtraction factor displayed next to the scroll bar; only the number of decimal places in the factor setting may be affected.

- To change the factor by typing a new value, choose Factor. In the dialog box that appears type a new factor in the text box and then choose OK, or choose Cancel if you don't want to change the factor.

#### 4. Choose Calculate.

The result spectrum appears in the bottom pane.

To expand or contract the Y-axis of the result spectrum, click the buttons to the right of the bottom pane. Expanding the spectrum helps you see small features.



Each time you click the Expand button, the scale of the Y-axis doubles.



Each time you click the Contract button, the scale is reduced by one-half.

#### 5. When you are satisfied with the result spectrum, you can replace the sample spectrum with it or add it to a spectral window.

To do this, select the desired option from the window selection box near the top of the Spectral Math window and then choose Add or Replace. The title of the spectrum will be Spectral Math Result.

To close the Spectral Math window without placing the result spectrum into a spectral window, click its Close button.

## Normalizing the frequency of a spectrum

Use Normalize Frequency in the Process menu to normalize the frequency of a displayed spectrum. This repositions the data points at standard locations; that is, the locations they would be at if they had been collected using a spectrometer with a reference laser frequency of 15,798.0 wavenumbers. This lets you compare spectra that were collected using spectrometers with different laser frequencies.

Normalize the spectra of your standards and unknown samples if you are developing or using a quantitative analysis method on more than one spectrometer. You should also normalize noncalibrated spectra; that is, JCAMP-DX spectra, spectra from CSV (comma-separated values) text files, and spectra collected using dispersive instruments.

The frequency is normalized only if it is not equal to the reference frequency and the difference between the two is less than 20 wavenumbers.

**Notice** Normalizing the frequency of spectra guarantees that data points occur at the same frequency positions. This lets you move data between spectrometers without the problems associated with inconsistent data point positioning. However, if you plan to analyze sample spectra using previously calibrated quant methods developed with a version of OMNIC earlier than 3.0, *do not normalize the frequency of the sample spectra*. If you normalize your sample spectra and attempt to use a calibrated method whose standards were not normalized, the data will not match and the analysis will fail. ▲

— **How to** ➔ Normalize the frequency of a spectrum

1. **Select the spectrum.**
2. **Choose Normalize Frequency from the Process menu.**

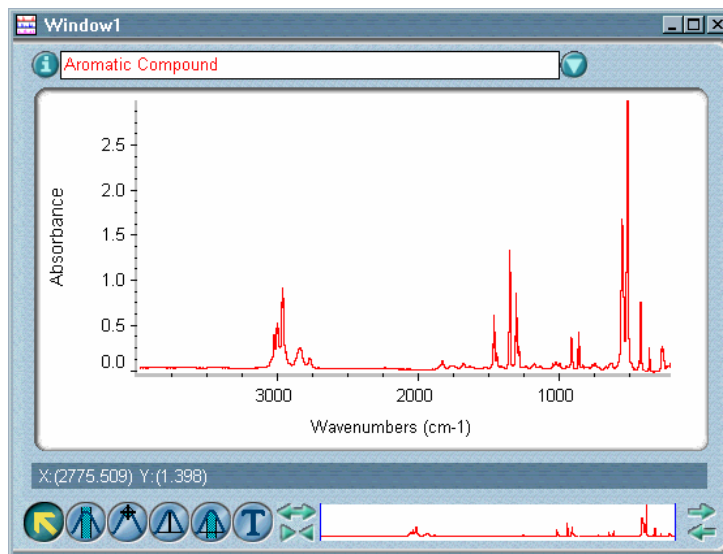
## Normalizing the scale of spectra

Use Normalize Scale in the Process menu to change the Y-axis scale of the selected spectra to a “normal” scale in which the Y values of the data points range from 0 absorbance units for the lowest point to 1 absorbance unit for the highest peak (for an absorbance or absorbance-like spectrum) or from 10% to 100% transmittance (for a transmission or transmission-like spectrum). These normal scales are typical of spectra in commercial spectral libraries.

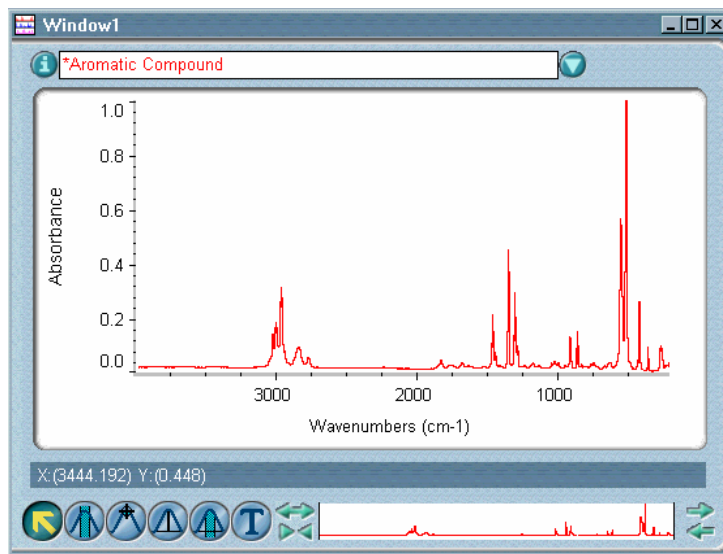
In a transmission experiment a thick sample of a material absorbs more infrared energy than a thin sample, resulting in greater peak heights. Normalizing the spectra compensates for this pathlength effect and lets you compare their peak heights.

In the case of an absorbance spectrum, Normalize Scale first shifts the spectrum vertically to bring the lowest Y value to 0 absorbance, regardless of whether the lowest value is currently above or below 0. The software then multiplies the spectrum by a scaling factor to make the highest value 1 absorbance unit.

Here is an example of an absorbance spectrum before being normalized:

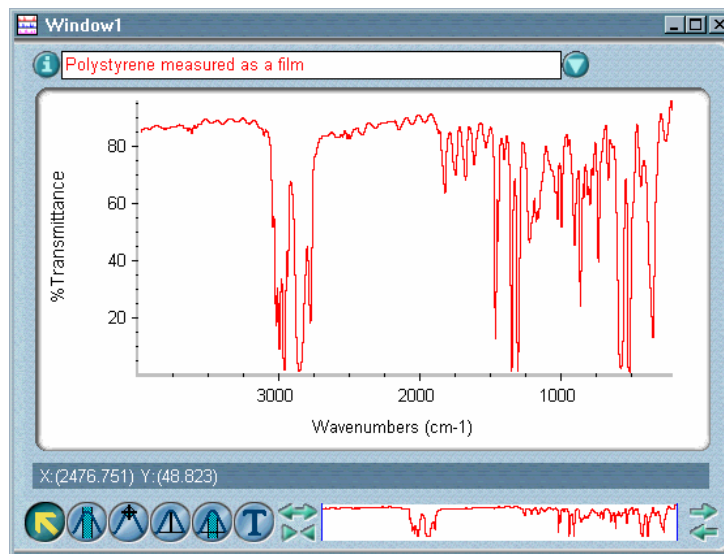


Here is the normalized spectrum:

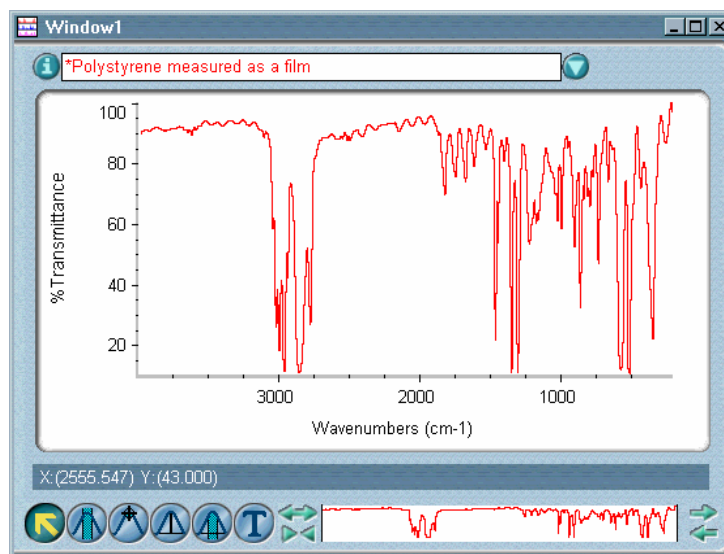


In the case of a transmission spectrum, the command first shifts the spectrum vertically to bring the highest Y value to 100 %T, regardless of whether the highest value is currently below or above 100%. The software then multiplies the spectrum by a scaling factor to make the lowest value (largest spectral feature) 10 %T.

The following example shows a spectrum before being normalized.



Here is the normalized spectrum:



The changes to the minimum and maximum Y values are recorded in the “DATA PROCESSING HISTORY” section of the Collection And Processing window.

**Notice** After a spectrum is normalized, you cannot use it for quantitative analysis unless you know the scaling factor and adjust the quantitative results accordingly. ▲

**■ *How to* ➔** Normalize the scale of spectra

- 1. Select the spectra.**
- 2. Choose Normalize Scale from the Process menu.**

# Analyze

Use the commands in the Analyze menu to obtain information from collected spectra. The primary use of each command is summarized in the following table:

To do this...	Use this command...
Identify peak locations in a spectrum.	Find Peaks
Export the selected spectra to OMNIC Spectra™ software.	Send To OMNIC Spectra
Measure noise in a spectrum.	Noise
Find the average Y value in a spectral region.	Average
Measure spectral variation within a group of spectra.	Statistical Spectra
Specify how to perform a spectral search or QC comparison.	Library Setup
Identify an unknown material by searching spectral libraries.	Search
Determine which chemical functional groups may be present in an FT-IR sample.	IR Spectral Interpretation
Verify the composition of a sample.	QC Compare
View spectral libraries and perform operations with them.	Library Manager
Add a spectrum to a user library.	Add To Library
Select a quantitative analysis method for quantifying a spectrum.	Quant Setup
Quantify a spectrum.	Quantify

If you are interested in performing quantitative analysis of your spectral data, see the documentation that came with your quant software for complete information.

You can customize the way OMNIC analyzes spectra by setting options using the Options command in the Edit menu. See “Customizing OMNIC by setting options” in the “Edit” chapter for details.

The next section describes the example spectral libraries provided with OMNIC. You can use these libraries to learn how to set up and perform a library search.

## Example libraries

The following sections describe the example libraries provided with your OMNIC software. These small libraries are subsets of libraries that you can purchase from us. If you are unfamiliar with using libraries, try the example libraries to learn how spectral searching and specific spectral libraries can be used to analyze data. Spectral searching is one of the most used analysis techniques in FT-IR spectroscopy. To see the contents of the libraries, use Library Manager in the Analyze menu. See “Managing libraries” later in this chapter for details.

A list of the compounds in the full reference libraries is provided with your OMNIC software. To view the list, plus other information about the reference libraries, click the Start button on the Windows taskbar, point to Programs (All Programs in Windows XP), point to the Thermo Scientific OMNIC folder, and then click the Library Listings item.

If you need more information about the reference libraries, contact us.

### **Aldrich Vapor Phase Sample Library**

All of the spectra in the Aldrich Vapor Phase Sample Library are also included in the complete Aldrich Vapor-Phase FT-IR Spectral Library. The complete library contains over 6,000 FT-IR spectra of compounds measured in the gas phase. The spectra were acquired by Aldrich Chemical Co. using samples of their products.

All of the Aldrich spectra are available in printed form in the *Aldrich Library of FT-IR Spectra*, Edition 1, Volume 3.



## **Georgia State Crime Lab Sample Library**

All of the spectra in the Georgia State Crime Lab Sample Library are also included in the complete Georgia State Forensic Drugs FT-IR Spectral Library. The complete library contains over 1,900 infrared spectra of drugs and drug-related compounds. The spectra were collected at  $4\text{ cm}^{-1}$  spectral resolution.

Samples include drugs, diluents, drug precursors and other drug-related compounds. Whenever possible, samples were secured as “pure” drug standards from the Drug Enforcement Administration (DEA), Applied Sciences Laboratories, United States Pharmacopeial Conventions, Inc., or various pharmaceutical companies. The sample purity was usually greater than 95% and, in many cases, the purity was greater than 99%.

## **Hummel Polymer Sample Library**

All of the spectra in the Hummel Polymer Sample Library are also included in the complete Hummel Polymers and Additives FT-IR Spectral Library. The complete library contains over 2,000 spectra of polymers, solvents, monomers and industrial organic compounds. The spectra were collected at the Institute of Physical Chemistry at the University of Cologne (Köln).

The library spectra were originally acquired at  $4\text{ cm}^{-1}$  spectral resolution. They were then mathematically deresolved when converted to Thermo Scientific library format.

## **Aldrich Condensed Phase Sample Library**

All of the spectra in the Aldrich Condensed Phase Sample Library are also included in the complete Aldrich FT-IR Collection, Edition 2 library. The complete library contains over 18,000 FT-IR spectra of substances, most of which are pure organic compounds.

The library spectra were originally acquired at  $2\text{ cm}^{-1}$  digital resolution and then mathematically deresolved when converted to Thermo Scientific library format.

Eight sublibraries of selected deresolved spectra from the complete Aldrich FT-IR Collection, Edition 2 library are also available from us. To see the titles and contents of the sublibraries, view the Library Listings item as described in the “Example libraries” section above.

## **Sigma Biological Sample Library**

All of the spectra in the Sigma Biological Sample Library are also included in the complete Sigma Biochemicals FT-IR Spectral Library. The complete library contains over 10,000 FT-IR spectra of interest to those in the biochemical field. The library spectra were originally acquired at  $2\text{ cm}^{-1}$  spectral resolution and then mathematically deresolved during conversion to Thermo Scientific library format.

Five sublibraries of selected deresolved spectra from the complete Sigma Biochemicals FT-IR Spectral Library are also available. To see the titles and contents of the sublibraries, view the Library Listings item as described in the “Example libraries” section above.

## **Organics by Raman Sample Library**

All of the spectra in the Organics by Raman Sample Library are also included in the complete Organics by FT-Raman Spectral Library. The complete library contains Raman spectra of 1,000 organic compounds.

The compounds in this library came from the 0-1000 MINI-STOCKROOM kit, which was obtained from Chem Service, Inc., of West Chester, Pennsylvania. The compounds arrived in brown glass bottles. Using a Thermo Scientific FT-Raman spectrometer, we were able to collect most of the spectra through the brown glass. The shipping bottles were not opened. A few of the compounds were provided in such small quantities that they had to be removed from the shipping bottles and sampled in NMR tubes.

The spectra have been Raman-shifted to wavenumber values to allow comparisons with infrared spectra. Your Raman sample spectra must be shifted before you used them to search this library.

## **User Example Library**

The 32-bit User Example Library contains 16 spectra from a variety of sources. The spectra have 4-wavenumber spectral resolution. This library is the only example library you can edit. Feel free to use this library to try the OMNIC search features. You can copy this library, edit the compound names, add or delete spectra from the library, and compress the library.

## **Finding peaks above a specified height**

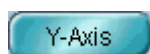
Use Find Peaks in the Analyze menu to identify peak locations in a spectrum. The command finds peaks in the displayed spectral region or in the selected region if you have selected one.

The command searches for peaks whose Y values exceed a specified threshold value and then labels them with their X values. A list of the peak locations is added to the log if you are currently logging operations.

By adjusting the threshold and sensitivity of the peak finding operation, you can find the spectral features you are interested in without labeling noise and other unimportant features.



Click the Print button in the Find Peaks window to print the spectrum and a table of the labeled peaks below it. The peaks are listed in the table in order of wavenumber position or Y value (intensity), depending on the order specified in the Process options (available through Options in the Edit menu).



If the Y-axis is not currently displayed in the window, you can display it by clicking the Y-Axis button. To remove the Y-axis from the window, click the button again.



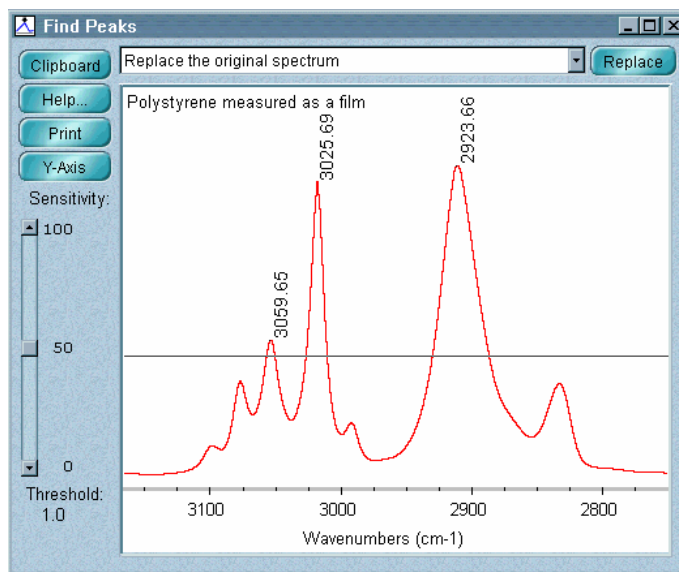
Click the Clipboard button in the Find Peaks window to copy a table of the labeled peaks to the Windows Clipboard. You can then paste the table into a word processing or spreadsheet program or other application that can accept text from the Clipboard.

You can use the annotation tool to edit the text of a peak label after you display the spectrum in a spectral window. The Annotation parameter in the Display Setup dialog box must be on to see the labels.

## Setting the threshold

The Threshold readout in the lower-left corner of the Find Peaks window shows the threshold, which is the Y value above which peaks can be found. (For a % transmittance spectrum, peaks below the threshold will be found.) For example, if the threshold value is 0.5, peaks in the selected spectral region whose Y value is greater than or equal to 0.5 will be found and labeled.

The threshold is represented by a horizontal line passing through the pane in the Find Peaks window (see the example below).



By changing the threshold value, you can find additional peaks or find fewer peaks. To change the threshold, click a point above or below the threshold line. The line moves to the level you clicked, and the new threshold value appears in the Threshold box. Set the threshold value equal to or slightly less than the Y value of the smallest peak you want to find.

## Setting the sensitivity

Use the scroll bar near the left side of the Find Peaks window to set the sensitivity. The sensitivity determines how readily Find Peaks finds shoulders on peaks and small peaks in the baseline. Unlike the threshold value, which merely specifies the Y value above which peaks are found, sensitivity takes into account the relative size of adjacent spectral features.

If you use a low sensitivity setting, a shoulder will be considered to be part of the larger peak and a small peak will be considered to be part of the noise in the baseline; neither feature will be found. At a higher sensitivity setting, the shoulder and small peak will be found and labeled as peaks.

If the sensitivity is set too high, noise and other unimportant features above the threshold will be found along with the useful features. Use a combination of threshold and sensitivity settings that lets you find just the spectral features you are interested in.

**■ How to ➡**

Find peaks in a spectral region or spectrum

- 1. Select the spectrum whose peaks you want to find and label.**
- 2. Display the spectral region in which you want to find peaks, or use the region tool to select a smaller region.**
- 3. Choose Find Peaks from the Analyze menu.**

The Find Peaks window appears. The peaks above the default threshold are labeled with their X values. For a % transmittance spectrum, peaks below the threshold are labeled. The threshold is indicated graphically by the horizontal line that runs through the spectrum. The exact threshold value appears in the Threshold box.

- 4. If you want to change the threshold value, click a point above or below the threshold line.**

The threshold line moves to the level you clicked, and the new threshold value appears in the Threshold box. The peaks above the new threshold are labeled with their X values, and peaks below the new threshold are not labeled. (For a % transmittance spectrum, peaks below the new threshold are labeled; peaks above the new threshold are not labeled.)

- 5. To change the sensitivity setting, use the Sensitivity scroll bar.**

The current setting is displayed to the right of the scroll bar. When you finish scrolling, any additional found peaks are labeled and peaks that are no longer found lose their labels.

- 6. To display or remove the Y-axis from the window, choose Y-axis.**
- 7. To print the spectrum and a table of the labeled peaks below it, choose Print.**

8. **To copy a table of the labeled peaks to the Windows Clipboard, choose Clipboard.**
9. **To replace the original spectrum with the labeled result spectrum or add the result to a spectral window, select the desired option from the window selection box at the top of the Find Peaks window and then choose Add or Replace.**

To close the Find Peaks window without placing the result spectrum into a spectral window, click its Close button. The results are added to the log when you close the window. If you save the result spectrum, the annotations also become part of the its collection and processing information and can be viewed in table form with the Annotation button.

## Exporting data to OMNIC Spectra

If you have installed OMNIC Spectra, you can export the selected spectra to that program by choosing Send To OMNIC Spectra from the Analyze menu. The spectra are added to the data tray. (If the spectra have not been saved, you are prompted to save them.) See the OMNIC Spectra Help system for complete information about analyzing the exported data

## Measuring noise

Use Noise in the Analyze menu to measure the noise in the selected spectral region of a spectrum (or in the displayed region if no region is selected). Both peak-to-peak and root mean square (rms) noise are measured.

The noise level of a spectrum depends on many factors, including the spectrometer, detector type, experiment parameter settings and the physical surroundings of the system.

Peak-to-peak noise is the difference between the highest and lowest noise peaks in the selected spectral region. Before measuring the noise, the software corrects any baseline tilt using a least-squares correction method.

An rms noise measurement is a statistical analysis of the noise variation. The rms noise level is equal to the square root of the average of the squares of the data points in the selected spectral region.

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

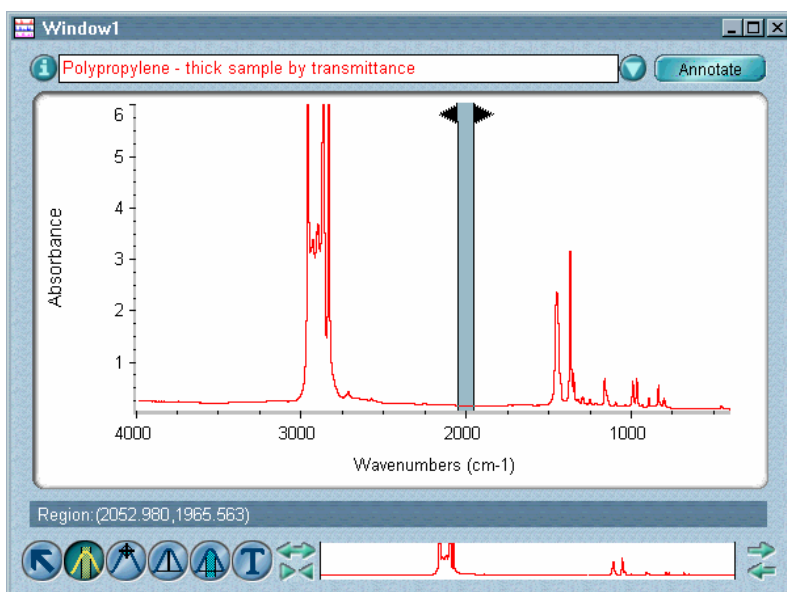
### — *How to* ➔

Calculate the noise in a spectral region or spectrum

1. **Select the spectrum.**
2. **Use the region tool to select a spectral region that has a flat baseline and no sample peaks.**

Any sample peaks in the region will be interpreted as noise and produce inflated results. A commonly used region is 2050 to 1950 wavenumbers. If you don't select a spectral region, the entire displayed region will be used to calculate the noise levels.

The following example shows a suitable region selected.



### 3. Choose Noise from the Analyze menu.

The Noise dialog box shows the peak-to-peak and rms noise levels and the X-axis limits of the region.

### 4. When you are finished viewing the noise level, choose OK.

The noise results are added to the log if you are currently logging operations and can be printed later.

## Finding the average Y value of a spectral region

### — How to —>

Use Average in the Analyze menu to find the average Y value of the data points in the selected spectral region of a spectrum (or in the displayed region if no region is selected).

Find the average Y value of a spectral region

#### 1. Select the spectrum you want to measure.

#### 2. Display or select the spectral region for which you want to find the average Y value.

The Average command works on the selected spectral region or on the currently displayed region if no region is selected. To select a spectral region, use the region tool. To display a spectral region, use the view finder, selection tool or Roll/Zoom window.

#### 3. Choose Average from the Analyze menu.

The Average dialog box shows the average Y value of the displayed or selected spectral region.

#### 4. Choose OK.



## Performing statistical calculations on spectra

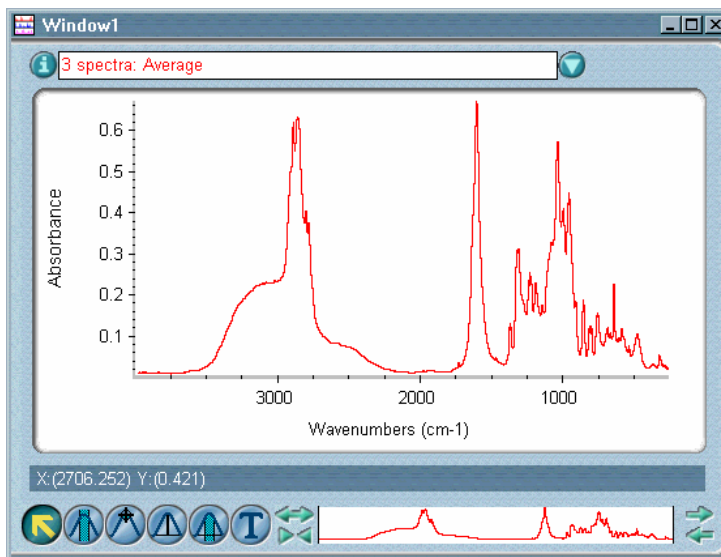
Statistical Spectra in the Analyze menu lets you perform statistical calculations on two or more selected spectra. For each data point (X value), you can find the average, variance and range of Y values for the spectra, as described in the following table.

Calculation	Description
Average	<p>The arithmetic mean of the Y values for each data point. (The Y values for a data point are added together, and then the total is divided by the number of spectra.)</p> <p>Possible uses: By calculating and saving the average of a group of spectra (of samples from a production run, for example), you can “average out” sample preparation and sampling variations. You can also use the average obtained from a group of standard samples as a reference (added to a search or QC library) that may be more representative of a compound than any single spectrum.</p>
Variance	<p>The standard deviation of the Y values for each data point. (The mathematical formula for standard deviation is used.)</p> <p>Possible uses: By comparing the variance of different peaks, you can detect the introduction of impurities in a production process. You can also calculate the variance of spectra of a standard sample collected at different times to check the repeatability of the spectrometer’s measurements.</p>
Range	<p>The range of Y values for each data point. (The lowest Y value for a data point is subtracted from the highest Y value for that point.)</p> <p>Possible uses: By comparing the ranges of groups of samples from different production runs, you can detect changes in how controlled a production process is. You can also compare the ranges obtained for a group of standard samples collected at different times to check the repeatability of the spectrometer’s measurements.</p>

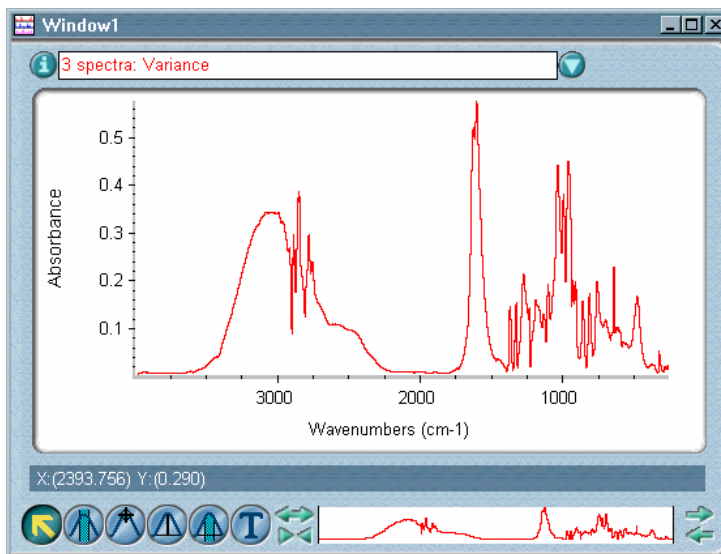
**Note** All the spectra must have the same X-axis and Y-axis units and the same data spacing. ▲

The results of the performed calculation are plotted in a spectral window using a vertical axis that indicates the average, variance or range and a horizontal axis that is identical to those of the original spectra. The default title given to each result spectrum is the number of spectra followed by the name of the calculation.

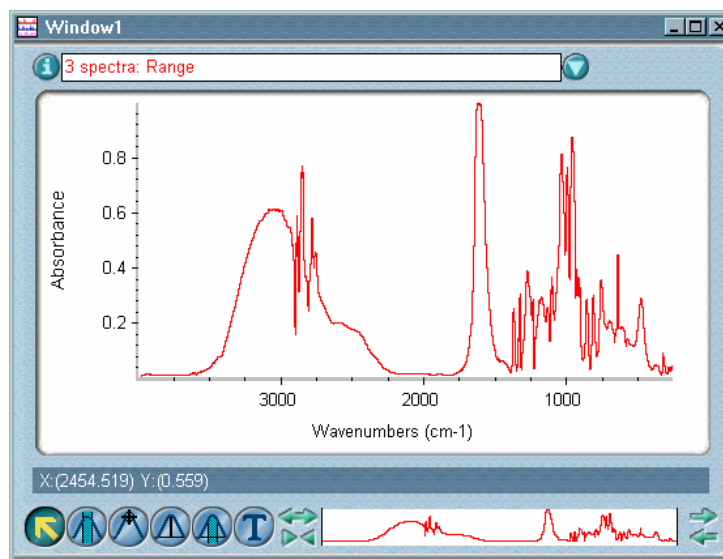
The following illustrations show examples of the results of each type of calculation.



Average of Y values versus X value



Variance of Y values versus X value



Range of Y values versus X value

### — *How to* ➔

Perform statistical calculations on a group of spectra

1. **Select the spectra.**
2. **Choose Statistical Spectra from the Analyze menu.**

The Statistical Spectra dialog box appears.

3. **Select the desired format of the data in the Data Format box.**

The spectra will be converted to the selected format before the calculations are performed. If you want the current Y-axis format of the spectra to be used, select Y-axis units. If you want the spectra converted to the first or second derivative, select First derivative or Second derivative, respectively.

4. **Select the calculations you want to perform by turning on the appropriate check boxes in the Save Format box.**
5. **Specify where to display the results by selecting an item from the drop-down list box at the top of the dialog box.**

## 6. Choose OK.

- If you specified that the results be added to an existing spectral window, the results are displayed in that window.
- If you selected Add To A New Window, and Prompt For New Window Title is turned on in the Window options, the New Window dialog box appears. Type a title for the spectral window and then choose OK. The results are then displayed in the new window.

## Setting up a spectral search or QC comparison

Use Library Setup in the Analyze menu to specify how to perform a spectral search of one or more search libraries to identify an unknown spectrum, or a QC comparison of one or more QC libraries to verify the composition of a sample.

Setting up a search or comparison consists of the basic steps described below. The features you need to perform these steps are on tabs in the Library Setup dialog box. To display a tab, click its name near the top of the dialog box. *Complete procedures for setting up a spectral search or QC comparison are provided later.* See “How to set up a spectral search” or “How to set up a QC comparison.”

### 1. Select the search libraries or QC libraries to include by using the Search Libraries tab or QC Libraries tab, respectively.

You can create groups of libraries whose spectra you can search or compare at one time. See “Selecting the libraries to include in a spectral search” and “Selecting the libraries to include in a QC comparison.”

You can specify library directories by using the Library Directories tab. (See “Selecting library directories” for details.) To save your directory specifications, use the Save Configuration As button.

### 2. If you are setting up a spectral search, use the Extended Search tab to specify whether and how to use the extended search feature.

This feature lets you add search criteria so that only spectra with a specified characteristic or that include particular text are found. The Extended Search tab does not affect QC comparisons. See “Using extended search” for details.

**3. If you are setting up a spectral search, specify the kind of search results you want using the Search Results tab.**

You can use the “search expert” or specify the search type (algorithm), number of spectra to find and a minimum match value. The Search Results tab does not affect QC comparisons. The search expert always searches the region from 2600 to 450 wavenumbers. See “Specifying the search results” for details.

**4. If you are not using the search expert (see step 3), specify the spectral regions of the library to include by using the Search Regions tab.**

See “Specifying the regions for a search or QC comparison” for details.



After you set up a spectral search, you can click the Search button or choose OK and then use Search in the Analyze menu to start the search. Similarly, after you set up QC comparison, you can click the QC Compare button or choose OK and then use QC Compare in the Analyze menu to start the comparison. See “Searching a spectral library” or “Performing a QC comparison” for complete instructions.

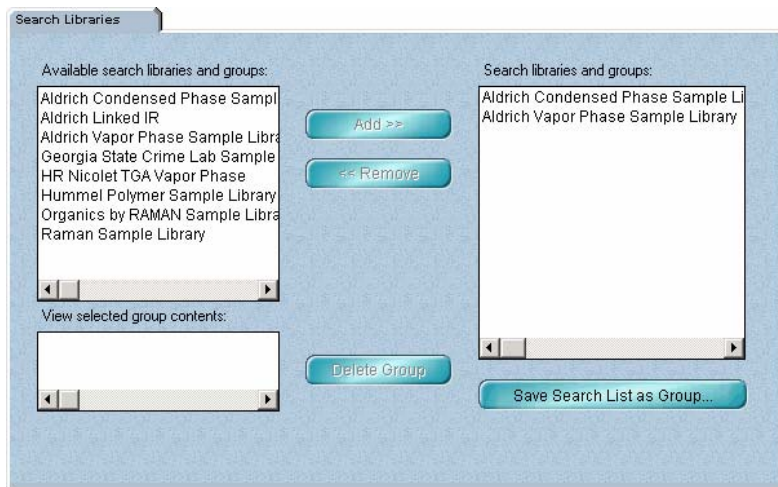
The library setup parameters are a subset of the parameters contained in the current experiment file. Any changes you make to the settings of the search and QC comparison parameters (except those on the Library Directories tab) will be saved when you save the experiment using the Save As button or using Experiment Setup in the Collect menu.

**Note** The parameter settings in the Library Setup dialog box (except those on the Library Directories tab) are automatically set when you select an experiment. ▲

You can obtain the best search and QC comparison results by properly preparing your sample and sample spectrum. See the tips provided later in this section.

## Selecting the libraries to include in a spectral search

The Search Libraries tab lets you specify the libraries to include when you perform a spectral search to identify an unknown spectrum.



If you frequently change your search libraries or often search particular libraries together, you can save time by linking them as a group. Once they are linked, you can move them in a single step to the list of libraries and groups to search.

The current library directories for both search libraries and QC libraries are listed in the Library Directories list box on the Library Directories tab.



All of the search libraries and search library groups in these directories are listed in alphabetical order in the Available Search Libraries And Groups box. If the libraries or groups you want to use are not listed, use the Add Directory button on the Library Directories tab to add the directories that contain them.




The libraries and groups currently selected for searching are listed in the Search Libraries And Groups box. Use the Add button to add the selected libraries or groups to this “search list” or the Remove button to remove them from the search list. Keep in mind that the more libraries and groups you include, the longer it will take to complete the search.

**Note** You can add or remove more than one library or group at a time by holding down the Control key when selecting the libraries or groups. ▲

When you select a group in the Available Search Libraries And Groups box, the libraries contained in the group are listed in the View Selected Group Contents box. (Scroll bars are provided when needed to scroll libraries into view.)



You can use the Save Search List As Group button to create a group containing all the libraries and groups in the search list in the Search Libraries And Groups box. You should normally group libraries only if they are similar or if you will frequently want to search them at the same time.



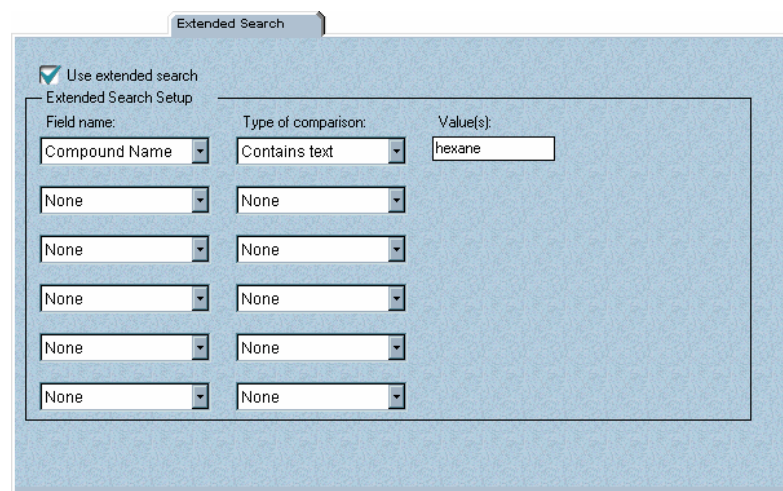
You can use the Delete Group button to remove the selected group from the list of available libraries and groups. The libraries remain on the hard disk but are no longer linked as a group.

To see a list of the compounds contained in a library, use Library Manager in the Analyze menu (see “Working with libraries” for details). To specify different default directories, use Options in the Edit menu (see “Specifying directories” in the “Edit” chapter for details).

## Using extended search

The Extended Search tab lets you specify whether and how to use extended search for spectral searches, including those performed by the search expert.

This tab does not affect QC comparisons.



Field name:	Type of comparison:	Value(s):
Compound Name	Contains text	hexane
None	None	
None	None	
None	None	
None	None	
None	None	

The extended search feature lets you include additional search criteria when you search a library to identify an unknown spectrum. This feature is typically used when some special characteristic or information about the spectrum is known and that type of information is contained in a “field” in the library. You can use only the Compound Name field and any custom information fields that are common to all the searched libraries. When you perform the search, only those library matches that meet the specified criteria—that is, have the specified information in the appropriate field—will be found and reported.

As an example, suppose that a library contains a field for indicating the name of a manufacturer and you want to search the library for spectra from a specific manufacturer. You first turn on Use Extended Search and then specify the manufacturer in the Extended Search Setup box. When you perform the search, only those library matches from that manufacturer are found. If ten matches would normally be found based on spectral information, but only four of those are from the manufacturer, then only four matches are reported.

The information needed for a comparison consists of the name of the field to be searched, the type of comparison and the text or values to search for.

**Note** If you search a library with extended search turned off, the special search criteria you specified for extended search will not be used. ▲

The following table describes the available comparison types and the additional text boxes that appear for each. The field names shown are just examples; your field names may be different. The available fields depend on which libraries are in the search list on the Search Libraries tab. To be available, a field must be contained in all the libraries in the search list and must be in the same position in the order of fields in all the libraries.

Comparison Type	Description
None	No comparison is performed for the field.
Contains Text	The field (or a portion of the field) must contain the text you specify in the Value(s) box.
Exact Text Match	The text in the field must exactly match the text you specify in the Value(s) box.



Comparison Type	Description
Numeric Range	The numeric value of the field must be within the range specified by the values you enter in the Value(s) boxes.

## Specifying the search results

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 and search results yourself. These options are on the Search Results tab. (This tab does not affect QC comparisons.)

Search Results

Use search expert  
 Configure search results

Search type: Correlation  Offset negative values

List of Matches

List compounds with match values above:

Maximum number of compounds in list:

Spectral Display

Number of library spectra to display:

Show match values

- If you turn on **Use Search Expert** on the Search Results tab, the search expert will determine the search algorithm to use and which regions to search.

The search algorithm affects how some spectral features and differences are weighed.

If you use the search expert, the spectral region you display or select in the spectral window and the spectral regions you specify on the Search Regions tab have no effect on the search. The search expert always searches the region from 2600 to 450 wavenumbers.

When you perform the search, the expert will display 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.

- If you turn on **Configure Search Results**, the Search Type drop-down list box and the features in the List Of Matches box become available (explained below). When you perform the search, the regions you specify will be used.

Specify the search type, or “algorithm,” for the search by selecting an option from the Search Type drop-down list box. The types described in the following table are available.

Search Type	Description
Correlation	Normally gives the best results and is recommended for most applications. The algorithm removes any effect of offset in the unknown spectrum, thus eliminating the effects of baseline variation.
Absolute Difference	Puts more weight on the small differences between the unknown spectrum and library spectra. This means that impurities will have a larger effect on the search results.
Squared Difference	Emphasizes the large peaks in the unknown spectrum. Use this algorithm if you are identifying a noisy spectrum.
Absolute Derivative	Gives small peaks and peak shifts an increased effect on the search results. The algorithm removes any differences between the unknown and library spectra caused by an offset in the unknown spectrum. This algorithm is useful when you want to emphasize peak positions rather than peak intensities. Use this algorithm if you are identifying a spectrum with a tilted baseline (and you don't want to correct the baseline before the search).

Search Type	Description
Squared Derivative	Emphasizes large peaks as well as peak shape. The algorithm removes any differences between the unknown and library spectra caused by an offset in the unknown spectrum. This algorithm works well with spectra of poor quality.

List Compounds With Match Values Above determines the minimum match value for searching and displaying results. Only those library spectra whose match value exceeds this number will be included in the list of matches. The maximum allowed setting is 100.

Maximum Number Of Compounds In List determines the maximum number of library spectra found. Enter a number just large enough to include all the spectra you expect to be similar to the unknown or the number of spectra you would be interested in viewing. Usually the default number of matches are enough to let you identify the unknown, if the library contains a good match. The maximum allowed setting is 500.

An unknown spectrum may contain data points with a negative absorbance value (or a Y value greater than 100% transmittance). OMNIC's search algorithms set these points to zero, which can lead to poor search results if the unknown has real spectral features with negative points. You can improve the results for these spectra by selecting Offset Negative Values. It offsets the entire spectrum so that all points are zero or above before normalizing the Y scale of the spectrum to match the scale of the library spectra (zero to one absorbance unit).

The features in the Spectral Display box let you specify how to display found library spectra. In the Number Of Library Spectra To Display text box type the maximum number of found library spectra you want displayed in panes in the search results. (You will be able to scroll spectra into view.) The maximum allowed setting is 100. If you want the match values of the spectra displayed in their panes, turn on Show Match Values.

### Specifying spectral regions for a search or QC comparison

When you perform a spectral search without using the search expert or perform a QC comparison, OMNIC performs the search or comparison on the entire spectrum or on the spectral region or regions you specify. The search expert always searches the region from 2600 to 450 wavenumbers.

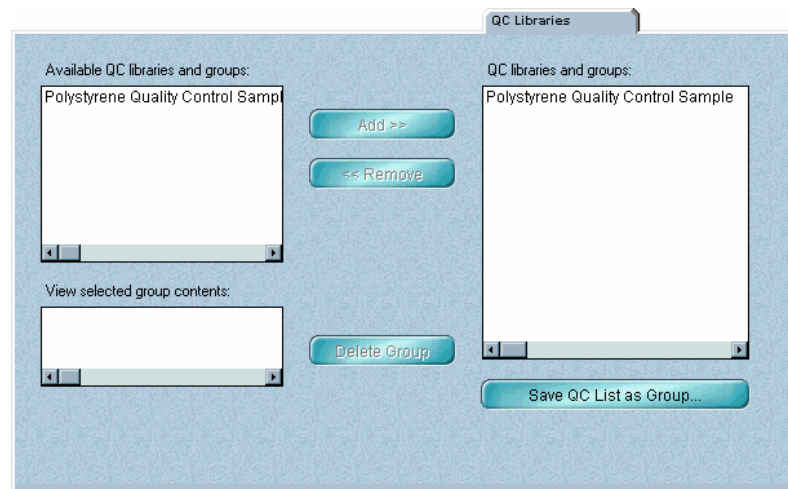
The regions for a spectral search or QC comparison are determined by three things:

- The regions you have specified for the library using the Search Regions tab in the Library Setup dialog box.
- Which regions were not blanked when you created the library.
- The region of the spectrum you have displayed or selected in the spectral window.

Only those portions of the spectrum which are within the selected region (or displayed region if no region is selected) *and* within the regions of the library that were not blanked *and* within any of the regions you specified for the library using the Search Regions tab will be included in the search or comparison.

## Selecting the libraries to include in a QC comparison

The QC Libraries tab lets you specify the spectral libraries to include when you perform a QC comparison to verify the composition of a sample.



If you frequently change the libraries you use or use particular libraries together, you can save time by linking them as a group. Once they are linked, you can move them in a single step to the list of libraries and groups to use for the comparison.

The current library directories for both search and QC libraries are listed in the Library Directories list box on the Library Directories tab.



All of the QC libraries and library groups in these directories are listed in alphabetical order in the Available QC Libraries And Groups box. If the libraries or groups you want to use are not listed, use the Add Directory button on the Library Directories tab to add the directories that contain them.



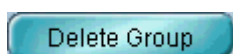
The libraries and groups currently selected for QC comparisons are listed in the QC Libraries And Groups box on the QC Libraries tab. Use the Add button to add the selected libraries or groups to this list or the Remove button to remove them from the list. Keep in mind that the more libraries and groups you include, the longer it will take to complete the comparison.

**Note** You can add or remove more than one library or group at a time by holding down the Control key when selecting the libraries or groups. ▲

When you select a group in the Available QC Libraries And Groups box, the libraries contained in the group are listed in the View Selected Group Contents box. (Scroll bars are provided when needed to scroll libraries into view.)



You can use the Save QC List As Group button to create a group containing all the libraries and groups listed in the QC Libraries And Groups box. You should normally group libraries only if they are similar or if you will frequently want to use them at the same time.

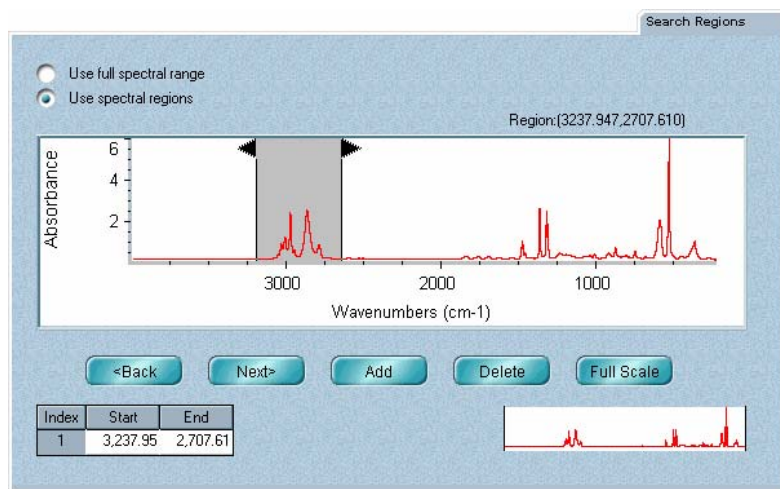


You can use the Delete Group button to remove the selected group from the list of available libraries and groups. The libraries remain on the hard disk but are no longer linked as a group.

To see a list of the compounds in a library, use Library Manager in the Analyze menu. To specify different default directories, use Options in the Edit menu.

## Specifying the regions for a search or QC comparison

The Search Regions tab lets you specify the spectral regions of the library that you want included in a spectral search or QC comparison.



For example, if a sample spectrum contains totally absorbing peaks, you should include only those regions that do not contain these peaks, since random noise at the top of these peaks will affect the search results.

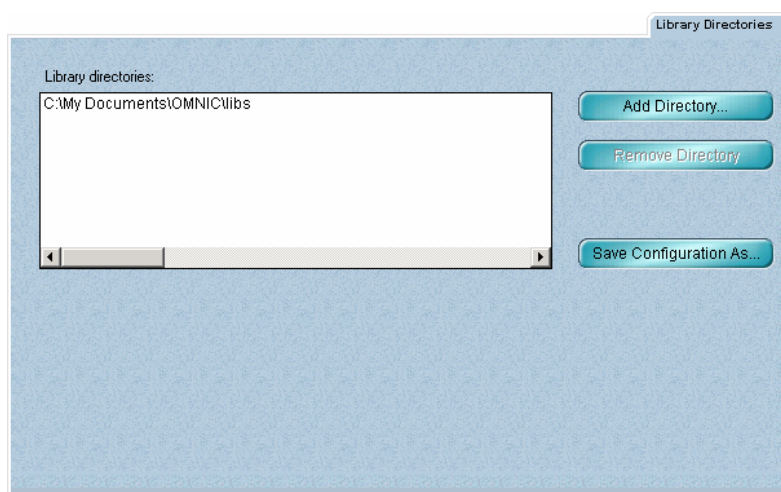
**Note** If you use the search expert for a search, the spectral regions you specify on the Search Regions tab or display or select in the spectral window have no effect on the search. The search expert always searches the region from 2600 to 450 wavenumbers. ▲

You can include the entire spectral range of the library in the search or comparison by selecting Use Full Spectral Range, or you can include just the specified spectral regions by selecting Use Spectral Regions. If you select the latter, use the rest of the features on the tab to specify the regions to include.

The spectral display pane shows the selected spectrum in red. Use this pane to specify graphically the regions to include. You can also specify a region by typing region limits in the table in the lower-left corner of the tab.

## Selecting library directories

The Library Directories tab lets you specify the spectral library directories for both search libraries and QC libraries. The current library directories are listed in the Library Directories list box. (Scroll bars are provided when needed to scroll directories into view.)



All of the libraries and library groups in these directories are listed in alphabetical order in the Available Search Libraries And Groups box on the Search Libraries tab and in the Available QC Libraries And Groups box on the QC Libraries tab. If the libraries or groups you want to use are not listed, use the Add Directory button on the Library Directories tab to add the directories that contain them.

### Note for DS systems

If Prevent Changing Directories When Opening Files is selected in the system policies, you cannot use the Add Directory button or Remove Directory button. ▲

You can use the Remove Directory button to remove a directory from the list (this does not remove the libraries from the disk).

### Note

If you remove the last directory from the list, it is replaced by the default directory specified on the File tab in the Options dialog box. ▲

To save your changes to the list of library directories in a configuration file, use the Save Configuration As button.

**— How to —>**

Set up a spectral search (The procedure for setting up a QC comparison follows this procedure.)

1. **If you want to specify spectral regions for the search graphically, select a spectrum you plan search.**
2. **Choose Library Setup from the Analyze menu.**

The Library Setup dialog box appears.

3. **On the Library Directories tab specify the directories that contain the libraries and library groups you want to search.**

To add a directory to the search list, choose Add Directory. In the dialog box that appears, locate and select the desired directory, and then choose Select.

**Note for DS systems**

If Prevent Changing Directories When Opening Files is selected in the system policies, you cannot use the Add Directory button or Remove Directory button. ▲

To delete a directory from the list, select it and then choose Remove Directory. (The directory remains on the hard disk; it is removed only from the list.)

**Note**

There must always be at least one directory in the list. If you remove the last remaining directory, the Initial User Library default directory specified in the File options (available through Options in the Edit menu) will be placed in the list. If you have the DS option, the directory specified by the Directory For User Libraries system policy will be placed in the list.) ▲

To save your changes to the list of library directories, use the Save Configuration As button. See the procedures in the “Saving a configuration” section in the “File” chapter if you need help.



#### 4. Specify the libraries and groups to search using the features on the Search Libraries tab.

To add one or more libraries or groups to the “search list” in the Search Libraries And Groups box, select the desired items in the list in the Available Search Libraries And Groups box and then choose Add. You can select more than one library or group at a time by holding down the Control key and clicking the desired items.

To see which libraries are contained in a group, select the group. The libraries it contains are listed in the View Selected Group Contents list box.

To remove one or more libraries or groups from the search list, select the items in the list and then choose Remove.

To delete a group from the list of available libraries and groups, select it and then choose Delete Group. The libraries contained in the group remain on the disk; only their association as a group is removed.

To create a group, set up the search list as described above and then choose Save Search List As Group. A message asks for a title for the group. Enter a title and then choose OK. A new group containing the libraries and groups in the search list is created and added to the list of available libraries and groups.

**Note** If more than one directory appears in the Library Directories box on the Library Directories tab when you create a group, the group is placed in the Initial User Library default directory specified in the File options (available through Options in the Edit menu). (If you have the DS option, the group is placed in the directory specified by the Directory For User Libraries system policy.) ▲

## 5. Use the Extended Search tab to specify whether and how to use the extended search feature.

To use extended search, first turn on Use Extended Search and then specify the needed information for each comparison you want performed:

- Specify the name of each library information field you want to search by selecting options from the Field Name drop-down list boxes.

If only one search library is specified on the Search Libraries tab, all the fields available in that library are listed. You can perform an extended search only on these fields. If more than one library is specified, the fields that appear depend on whether the fields in all the specified libraries are identical and in the same order. If they are, then all the available fields appear. If the fields are not identical or not in the same order, then only the Compound Name field appears.

You can search up to six fields. Only those spectra whose field information matches the search information you enter will be found and reported by the extended search.

- For each specified field, specify how to compare the information in the field with the search information by selecting an option from the Type Of Comparison drop-down list box.
- Type the text or values to search for in the text box or boxes that appear when you select a comparison type.

**Note** If you search a library with extended search turned off, the special search criteria you specify in this procedure will not be used. ▲

**6. Specify the kind of search results you want by clicking the Search Results tab and setting the parameters.**

If you want the search performed by the search expert, select Use Search Expert and go to the next step. (If you use the search expert, the spectral regions you specify on the Search Regions tab or display or select in the spectral window have no effect on the search. The search expert always searches the region from 2600 to 450 wavenumbers.) If you want to specify the search results, select Configure Search Results and then set the parameters that become available:

- Specify the search type by selecting an algorithm from the Search Type drop-down list box.
- Specify the minimum match value for searching and displaying results by typing a number in the List Compounds With Match Values Above text box.
- Specify the maximum number of library spectra to find and list by typing a number in the Maximum Number Of Compounds In List text box.

**7. Specify the number of found library spectra to display at one time in the search results panes by typing a number in the Number Of Library Spectra To Display text box.**

You can scroll other found library spectra into view if there are more spectra than panes.

**8. If you want the match values of the library spectra displayed in their panes, turn on Show Match Values.**

**9. If you are not using the search expert (see step 5), specify the spectral regions to include in the search by clicking the Search Regions tab.**

If you want the entire spectral range of the library to be searched, select Use Full Spectral Range and go to the next step.

To search only spectral regions you specify, select Use Spectral Regions.

Specify the first spectral region you want search. You can do this graphically or by typing region limits in the table in the lower-left corner of the tab. To make it easier to specify regions, you can use the view finder to expand the spectral display. You can also click the Full Scale button to display the spectrum full scale at any time.

- To specify the region in the spectral display pane, point to where you want the region to start, press and hold down the mouse button, move the pointer where you want the region to end, and then release the mouse button. The specified region is shaded and bordered by vertical lines. The limits of the region appear above the pane and in the table in the lower-left corner of the tab. You can change the region limits by dragging the triangular handles on the vertical lines that border the region.
- To specify the region using the table, click the cell below Start and type the desired starting limit of the region. Click the cell below End and type the desired ending limit. You can press Enter to enter a value you typed. The entered values are reflected by the size and location of the shaded region in the pane and the readout of region limits above the pane.

After you have specified a region, choose Add. The Index number in the table increases by one, and you can now specify the next region.

Specify the other regions you want searched in the same manner.

You can view the regions you have specified by using the Back and Next buttons to display the preceding or next region in the pane, respectively.

**10. Choose OK to close the dialog box, or choose Search to start the spectral search immediately.**

The selected spectrum will be searched against the specified libraries. If you choose OK, you can start a spectral search by choosing Search from the Analyze menu. Choose Cancel if you don't want your changes to the parameters saved.

See “Searching a spectral library” for details on how a spectral search is performed and how the results are displayed.

**Note** To save your changes to the library setup parameters (except those on the Library Directories tab), use the Save As button to save the experiment. Each time you open the experiment, the parameters will be set automatically. To save your library directory specifications, use the Save Configuration As button on the Library Directories tab. ▲

**— How to ➔** Set up a QC comparison (The procedure for setting up a spectral search precedes this procedure.)

**1. If you want to specify spectral regions for the comparison graphically, select a spectrum you plan to compare.**

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

The Library Setup dialog box appears.

**3. On the Library Directories tab specify the directories that contain the libraries and library groups you want to include in the comparison.**

To add a directory to the list of directories, choose Add Directory. In the dialog box that appears, locate and select the desired directory, and then choose Select.

**Note for DS systems** If Prevent Changing Directories When Opening Files is selected in the system policies, you cannot use the Add Directory button or Remove Directory button. ▲

To delete a directory from the list, select it and then choose Remove Directory. (The directory remains on the hard disk; it is removed only from the list.)

**Note** There must always be at least one directory in the list. If you remove the last remaining directory, the Initial User Library default directory specified in the File options (available through Options in the Edit menu) will be placed in the list. (If you have the DS option, the directory specified by the Directory For User Libraries system policy will be placed in the list.) ▲

To save your changes to the list of library directories, use the Save Configuration As button. See the procedures in the “Saving a configuration” section in the “File” chapter if you need help.

**4. Click the QC Libraries tab and use its features to specify the libraries and groups to include.**

To add one or more libraries or groups to the list in the QC Libraries And Groups box, select the desired items in the list in the Available QC Libraries And Groups box and then choose Add. You can select more than one library or group at a time by holding down the Control key and clicking the desired items.

To see which libraries are contained in a group, select the group. The libraries it contains are listed in the View Selected Group Contents list box.

To remove one or more libraries or groups from the list in the QC Libraries And Groups box, select the items in the list and then choose Remove.

To delete a group from the list of available libraries and groups, select it and then choose Delete Group. The libraries contained in the group remain on the disk; only their association as a group is removed.

To create a group, set up the list of libraries and groups for the comparison as described above and then choose Save QC List As Group. A message asks for a title for the group. Enter a title and then choose OK. A new group containing the libraries and groups in the list is created and added to the list of available libraries and groups.

**5. Specify the spectral regions to include in the comparison by clicking the Search Regions tab.**

If you want the entire spectral range of the library to be included, select Use Full Library Range and go to the next step.

To include only spectral regions you specify, select Use Spectral Regions.

Specify the first spectral region you want to include. You can do this graphically or by typing region limits in the table in the lower-left corner of the tab. To make it easier to specify regions, you can use the view finder to expand the spectral display. You can also click the Full Scale button to display the spectrum full scale at any time.

- To specify the region in the spectral display pane, point to where you want the region to start, press and hold down the mouse button, move the pointer where you want the region to end, and then release the mouse button. The specified region is shaded and bordered by vertical lines. The limits of the region appear above the pane and in the table in the lower-left corner of the tab. You can change the region limits by dragging the triangular handles on the vertical lines that border the region.
- To specify the region using the table, click the cell below Start and type the desired starting limit of the region. Click the cell below End and type the desired ending limit. You can press Enter to enter a value you typed. The entered values are reflected by the size and location of the shaded region in the pane and the readout of region limits above the pane.

After you have specified a region, choose Add. The Index number in the table increases by one, and you can now specify the next region.

Specify the other regions you want included in the same manner.

You can view the regions you have specified by using the Back and Next buttons to display the preceding or next region in the pane, respectively.

**6. Choose OK to close the dialog box, or choose QC Compare to start the QC comparison immediately.**

The selected spectrum will be compared with the spectra in the specified libraries. If you choose OK, you can start a QC comparison by choosing QC Compare from the Analyze menu. Choose Cancel if you don't want your changes to the comparison parameters saved.

See “Performing a QC comparison” for information on QC comparisons.

**Note** To save your changes to the comparison parameters (except those on the Library Directories tab), use the Save As button to save the experiment. Each time you open the experiment, the parameters will be set automatically. To save your library directory specifications, use the Save Configuration As button on the Library Directories tab. ▲

## Searching a spectral library

Use Search in the Analyze menu (or the Search button in the Library Setup dialog box) to identify an unknown material. Search compares the unknown sample spectrum with each reference spectrum in the libraries selected using Library Setup and finds the spectra that most closely match the unknown. (See “Setting up a spectral search or QC comparison” for complete information on selecting libraries and setting the search parameters.)

**Note** If you just want to verify the composition of a sample, you can use QC Compare in the Analyze menu. See “Performing a QC comparison” for details. ▲

You can include the entire unknown spectrum in the search or just certain spectral regions. The searched regions are determined by the following things:

- Which regions you have specified for the library using the Search Regions tab in the Library Setup dialog box. See “Specifying the regions for a search or QC comparison” for details.
- Which region of the unknown spectrum you have displayed or selected in the spectral window.
- The intersection of the spectral ranges of the libraries being searched: A spectral region is searched only if it is within the spectral ranges of all the included libraries.
- Which regions were not blanked when the library was created. See “Creating a user library” for more information.

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 Search Regions tab will be included in the search.



The way the search results are displayed after the search depends on how you set up the search using the Search Results tab in the Library Setup dialog box. For example, if you specified that the search expert be used, the list of library matches does not appear unless you click the View Match List button.

If the list of matches is displayed, it shows for each match the library index number, a match value between 0 and 100, the compound name and the name of the library that contains the match. The match value tells you how well the library spectrum matches the unknown. A match value of 100 indicates a perfect match. The closer the value is to 100, the better is the match.



You can use the Info button to see information about one or more matches in the list. When you choose Info, a dialog box shows information about the first selected match. To see information about the next selected match, choose Next. To see information about the previous match, choose Previous. When you are finished viewing the information, choose Close.

If you use the search expert, comments about the search results appear in the lower portion of the Search window.

If you want to change how the search results are displayed, choose Modify Display. You will be able to specify the number of found library spectra to display at one time, specify that match values be displayed in the spectra's panes, or change the number of compounds shown in the list.

When an exact match is not found, several library spectra may resemble the unknown spectrum to a similar degree. You can compare the best matches visually with the unknown spectrum before deciding which is the closest match.

### ■ *How to* ➔

Search a spectral library

1. **Use Library Setup in the Analyze menu to set up the search.**
2. **Select the spectrum that you want to identify.**

**3. If desired, specify a spectral region to search by selecting it with the region tool or by displaying it in the spectral window.**

**If you are not using the search expert**, the searched spectral regions are determined by the following things:

- Which regions you have specified for the library using the Search Regions tab in the Library Setup dialog box.
- Which region of the unknown spectrum you have displayed or selected in the spectral window.
- The intersection of the spectral ranges of the libraries being searched: A spectral region is searched only if it is within the spectral ranges of all the included libraries.
- Which regions were not blanked when the library was created.

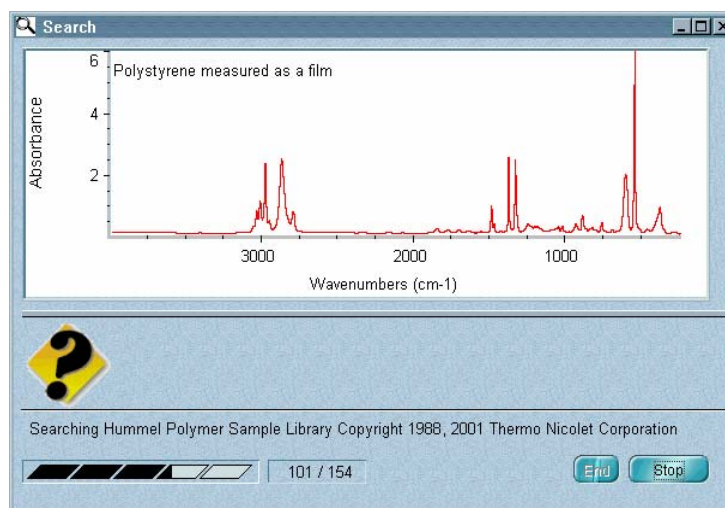
Only those portions of the spectrum which are within the selected region (or displayed region if no region is selected) *and* within any of the regions you specified for the library using the Search Regions tab will be included.

Use Blank in the Process menu to delete any peaks you want excluded, or just search a region that doesn't contain the peaks. When searching a mixture spectrum, search a region that contains peaks from one of the components.

**If you are using the search expert**, the regions you specify on the Search Regions tab or display or select in the spectral window have no effect on the search. The search expert always searches the region from 2600 to 450  $\text{cm}^{-1}$ .

#### 4. Choose Search from the Analyze menu.

The Search window appears:



**Note** You can also start a search by clicking the Search button in the Library Setup dialog box immediately after setting up the search (as in step 1). ▲

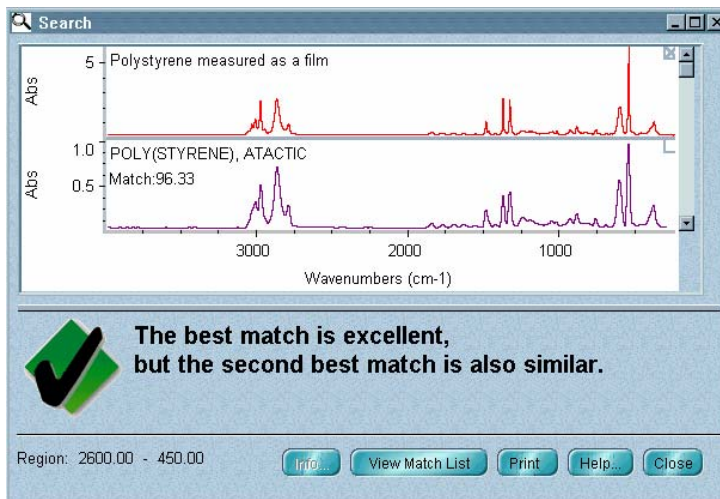
At the bottom of the window a gauge shows the progress of the search. The number of library spectra searched so far is shown to the left of the total number of library spectra included in the search. The name of the library being searched appears above the gauge.

As library matches are found, the closest matches are added to the search results list (if it is displayed) in order of match value, with the best match listed first.

To interrupt the search before it is complete, choose Stop. The matches found so far are listed, and the Stop button becomes the Resume button. To continue the search, choose Resume. As additional matches are found, they are added to the list. You can stop and resume the search as many times as you like.

If you don't want to continue after stopping the search, choose End.

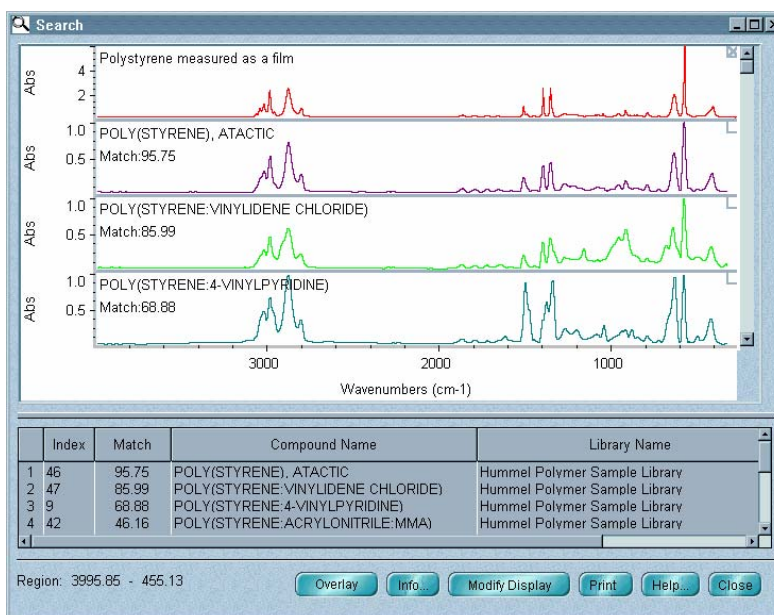
When the search is finished, the limits of the selected spectral region (or displayed region if no region is selected) appear in the lower-left corner of the window (see the following example). If you did not use the region tool or view finder to specify a region to search, the limits of the entire spectrum appear.



The unknown spectrum and found library spectra are displayed in panes in the upper portion of the window. You can drag the horizontal bar that is below the panes down or up to allocate more or less space for displaying the spectra. Use the scroll bar to the right of the panes to display spectra that are out of view.

If you turned on Show Match Values on the Search Results tab in the Library Setup dialog box before the search, you can click a spectrum to see its match value. To return to the stacked display, choose Stack Spectra from the View menu.

If you did not use the search expert, a list of the library matches appears in the lower portion of the window.



To overlay a library spectrum and the unknown, click the Overlay button and select the desired spectrum in the list (if it is displayed). The Overlay button becomes the Stack button. Click it if you want to return to the stacked display.

**5. You can see additional information about one or more matches in the list (if it is displayed).**

One way to do this is to select the matches and then choose Info. To select a match, click it. To select an additional match, hold down the Control key and click the match. You can select several adjacent matches by clicking the first match and then holding down the Shift key and clicking last match.

When you choose Info, a dialog box shows information about the first selected match. To see information about the next selected match, choose Next. To see information about the previous match, choose Previous. When you are finished viewing the information, choose Close.

If you searched a user library for which you have drawn and saved chemical structures using the Create/Edit Structures button on the Library Spectra tab of Library Manager, you can display the structure for a match by selecting it in the list. The structure appears in a small window that you can position as desired. The window title shows the name of the compound. The index number (ID) of the spectrum and the chemical formula and molecular weight (MW) of the compound appear at the bottom. If the window is empty, no structure has been drawn for that spectrum. See “Drawing or editing chemical structures.”

**6. If you want to change how the search results are displayed, choose Modify Display.**

The Modify Search Display dialog box appears. Specify the number of found library spectra to display at one time by typing a number in the Number Of Library Spectra To Display text box. (You can scroll other found library spectra into view if there are more spectra than panes.)

If you want the match values of the library spectra displayed in their panes, turn on Show Match Values.

If you want to change the number of compounds shown in the match list, type a value in the Number Of Compounds In Match List text box. The maximum allowed value is the number of matches found.

When you are finished, choose OK.

## 7. To print the search results on paper, choose Print.

The Print dialog box appears.

To print the spectra, turn on Search Results Spectra.

To print any structure you have drawn and saved with the spectrum, turn on Structure Diagram. (This option appears only if you didn't use the search expert.)

To print the search expert's comments, turn on Search Expert's Comments. (This option appears only if you used the search expert.)

To print the list of matches, turn on Search Results List Of Matches.

If you want each spectrum and the list of matches to be printed on separate pages, turn on Print Items On Separate Pages.

To set up the printer, choose Printer Setup. The Print Setup dialog box appears. Select the printer from the list box. You can also specify portrait or landscape page orientation.

**Note** If you change the orientation, the Orientation option in the Print options (available through Options in the Edit menu) will be reset to the new orientation. The page orientation setting in Windows Control Panel or in the printer setup dialog box for other applications is not affected by the setting you make here. ▲

If you want to set the printer parameters, choose Properties in the Print Setup dialog box. If you don't want to set the parameters, choose OK. If you choose Properties, a dialog box shows the current settings of the printer parameters. This dialog box varies in appearance depending on your printer. See the documentation that came with your printer for information on setting the printer parameters. After you set the parameters, choose OK to close the dialog box, and then choose OK to close the Print Setup dialog box.

When you are ready to start printing, choose OK.

**8. To copy the search results to the Windows Clipboard, click the Clipboard button.**

You can then paste the results into a program that can accept text from the Clipboard.

**9. To close the Search window, choose Close.**

You can start another search without closing this window. You will not be able to change what is displayed in the first Search window, but you will be able to print its contents.

## **Finding functional groups**

Use IR Spectral Interpretation in the Analyze menu to help you determine which chemical functional groups may be present in an FT-IR sample. The command examines the frequency locations and intensities of peaks in the sample spectrum, or in a specified spectral region, and then lists the functional groups that may be present, along with reference information about the groups. Use this information along with your own evaluation of the spectrum to determine which functional groups are actually present in the sample.

No special preparation is needed before you use this command to find functional groups in a spectrum. However, keep in mind that the presence of totally absorbing bands in a sample spectrum may reduce the accuracy of the results.

## — How to → Find for functional groups

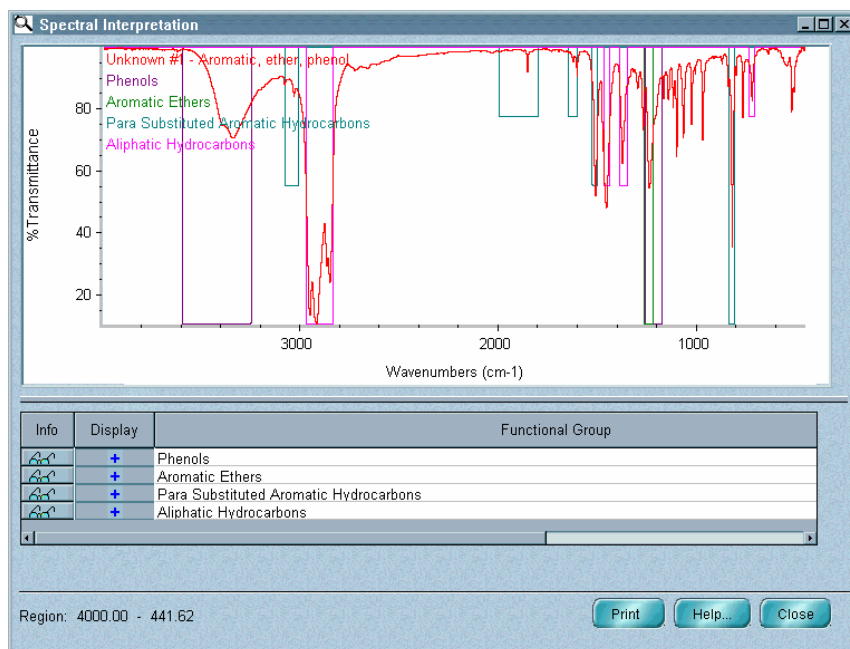
1. **Select the spectrum you want to examine.**
2. **If desired, specify a spectral region to examine by selecting it with the region tool or by displaying it in the spectral window.**
3. **Choose IR Spectral Interpretation from the Analyze menu.**

The Spectral Interpretation window appears showing the spectrum in % transmittance units. A gauge in the lower-left corner of the window shows the progress of the interpretation.

You can interrupt the interpretation by choosing Stop. The Stop button becomes the Resume button, and the End button appears. To resume the interpretation, choose Resume. If you want to end the interpretation at this point, choose End.

When the interpretation is complete, the limits of the examined region appear in the lower-left corner of the window. A pane at the top of the window shows the entire sample spectrum, plus the functional group bands that may be present in the sample.

Here is an example:





Color-coded titles of the spectrum and functional group bands appear in the upper-left corner. The peaks in the functional group bands are squared off to more simply represent the locations and typical intensities of the bands.

The found functional groups are listed in the Functional Group column of the table below the pane. In the Display column you can click the plus (+) sign next to a functional group title to turn off the display of that functional group in the pane. Click that row in Display column again to display the functional group bands again; the plus sign reappears. Displaying only the functional groups of interest can make it easier to interpret the results. If needed, a scroll bar is provided at the right side of the table to allow you to scroll titles into view.

At the left end of the table are Info buttons that you can click to see reference information about the found functional groups. When you click the Info button for a functional group, Microsoft Internet Explorer (or your default web browser) starts and displays the corresponding reference information.

Use the scroll bar at the right side of the window to scroll information into view. You can print the information by using the Print command in the File menu of Internet Explorer. When you are finished, close Internet Explorer by choosing Close from its File menu.

You can drag the horizontal bar below the pane of the Spectral Interpretation window up or down to allocate more or less space for displaying the pane and the table.

#### **4. To print the results, choose Print.**

The Print dialog box appears. To print the spectrum and functional group bands, turn on IR Spectral Interpretation Results Spectra. To print the contents of the table, turn on IR Spectral Interpretation Table.

You can use the Printer Setup button to set parameters that affect how the information will be printed; for example, the printer or paper orientation to use.

When you are finished, choose OK.

5. When you are finished viewing the results, choose **Close** to close the **Spectral Interpretation** window.

## Performing a QC comparison

Use QC Compare in the Analyze menu to verify the composition of a sample. The command compares the spectrum of the sample with spectra in the specified QC libraries and reports how well the spectrum matches the library spectra.

The spectra in a QC library are not independent (as in a search library) but instead are grouped into compound types. Because of this, the result of comparing a sample spectrum with the spectra in a QC library is not a list of the best individual matches in the library but instead a display of the single best match from each type.

**Note** If you want to identify an unknown spectrum, use Search in the Analyze menu. See “Searching a spectral library” for details. ▲

You can include the entire sample spectrum in the comparison or just certain spectral regions. The compared regions are determined by three things:

- The regions you have specified for the library using the Search Regions tab in the Library Setup dialog box.
- Which regions were not blanked when you created the library.
- The region of the spectrum you have displayed or selected in the spectral window.

Only those portions of the spectrum which are within the selected region (or displayed region if no region is selected) *and* within the regions of the library that were not blanked *and* within any of the regions you specified for the library using the Search Regions tab will be included in the comparison.

### ■ *How to* ➔

Perform a QC comparison

1. Use **Library Setup** in the **Analyze** menu to set up the **QC comparison**.

2. **Select the spectrum whose composition you want to verify.**
3. **If desired, specify a spectral region to compare by selecting it with the region tool or by displaying it in the spectral window.**

The compared regions are determined by the following things:

- Which regions you have specified for the library using the Search Regions tab in the Library Setup dialog box.
- Which regions were not blanked when you created the library.
- Which region of the sample spectrum you have displayed or selected in the spectral window.
- The intersection of the spectral ranges of the libraries being searched: A spectral region is searched only if it is within the spectral ranges of all the included libraries.

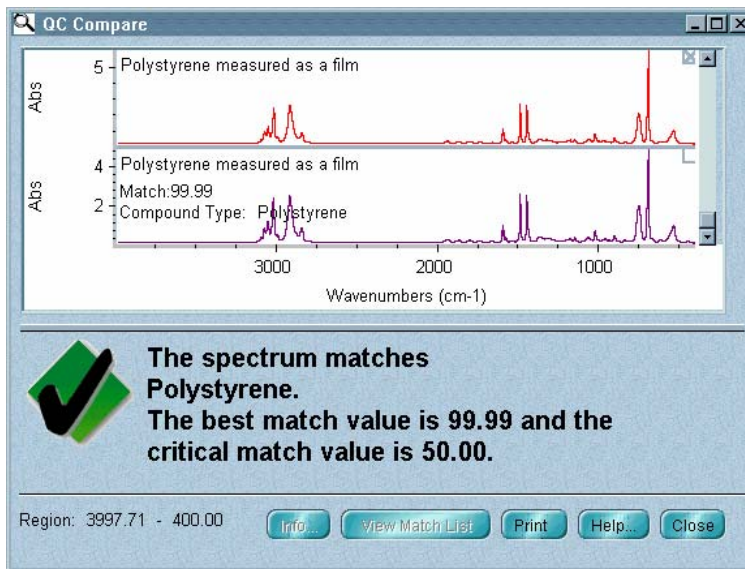
Use Blank in the Process menu to delete any peaks you want excluded, or just include a region that doesn't contain the peaks. When comparing a mixture spectrum, include a region that contains peaks from one of the components.

4. **Choose QC Compare from the Analyze menu.**

The QC Compare window appears. At the bottom of the window a gauge shows the progress of the comparison. The number of library spectra compared so far is shown to the left of the total number of library spectra included in the comparison. The name of the library being compared appears above the gauge.

To interrupt the comparison before it is complete, choose Stop. The results found so far are shown, and the Stop button becomes the Resume button. To continue the comparison, choose Resume. You can stop and resume the search as many times as you like. If you don't want to continue after stopping the comparison, choose End.

When the comparison is finished, the limits of the selected spectral region (or displayed region if no region is selected) are displayed in the lower-left corner of the window. If you did not use the region tool or view finder to specify a region to compare, the limits of the entire spectrum are displayed.



The sample spectrum and the library spectrum that best matches it are displayed in panes in the upper portion of the window. You can drag the horizontal bar that is below the panes down or up to allocate more or less space for displaying the spectra. You can use the scroll bar to the right of the panes to display any spectra that are out of view. These are the spectra in the other compound types that best match the sample spectrum.

You can choose **Overlay Spectra** from the **View** menu to display the spectra overlaid. If you turned on **Show Match Values** on the **Search Results** tab in the **Library Setup** dialog box before the comparison, you can click a spectrum to see its match value. To return to the stacked display, choose **Stack Spectra** from the **View** menu.

Comments about the comparison results appear in the lower portion of the window. If a match is found, the comments tell you which compound type the sample spectrum most closely matches.

**Note** The **Info** and **Modify Display** buttons are not available for a **QC** comparison. ▲

**5. To print the comparison results on paper, choose Print. The Print dialog box appears.**

If you want to print the spectra, turn on QC Compare Spectra.

If you want to print the comments, turn on QC Compare Comments.

If you want each spectrum and the list of matches to be printed on separate pages, turn on Print Items On Separate Pages.

To set up the printer, choose Printer Setup. The Print Setup dialog box appears. Select the printer from the list box. You can also specify portrait or landscape page orientation.

**Note** If you change the orientation, the Orientation option in the Print options (available through Options in the Edit menu) will be reset to the new orientation. The page orientation setting in Windows Control Panel or in the printer setup dialog box for other applications is not affected by the setting you make here. ▲

If you want to set the printer parameters, choose Properties in the Print Setup dialog box. If you don't want to set the parameters, choose OK. If you choose Properties, a dialog box shows the current settings of the printer parameters. This dialog box varies in appearance depending on your printer. See the documentation that came with your printer for information on setting the printer parameters. After you set the parameters, choose OK to close the dialog box, and then choose OK to close the Print Setup dialog box.

When you are ready to start printing, choose OK.

**6. To close the QC Compare window, choose Close.**

## Managing libraries

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. You can browse through a library one spectrum at a time or use the text search feature to find spectra whose associated information contains specified text.

**Note** Listings of the spectra contained in commercial libraries are available on our web site: Go to [www.thermo.com](http://www.thermo.com), use Search near the top of the page to find "libraries" and then click the name of the library you are interested in. The Downloadable Files section on the resulting page contains a link for displaying the PDF listing for that library, if available. ▲

Library Manager contains four tabs, each labeled at the top. When you click a tab, its information and features are brought to the front.

The **Library Names** tab lets you view the titles of the spectra contained in your libraries and perform these operations:

Create a new user library. See "Creating a user library."

Add all the spectra in one user library to another (merge two user libraries). See "Merging user libraries."

Renumber the spectra in a user library (compress the library) to eliminate empty slots created when spectra were removed. See "Compressing a user library."

Place a copy of a library spectrum into a spectral window. See "Placing a library spectrum into a spectral window."

Place a copy of a user library spectrum into another user library. See "Adding user library spectra to another user library."

Delete a user library spectrum from a user library. See "Deleting a spectrum from a user library."

Delete a user library. See "Deleting a user library."

Collect a sample spectrum and place it into a user library. See "Collecting a spectrum and adding it to a user library."

List the spectra in a library in order by index number, title or date of addition to the library. See "Working with libraries."

Sign a user library. See "Signing a user library."

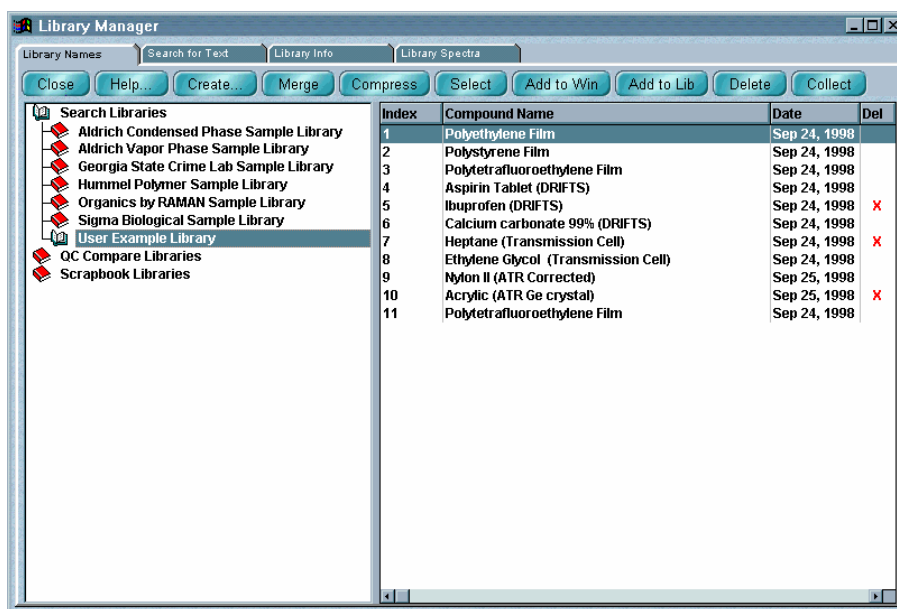
The **Search For Text** tab lets you find library spectra by searching for an index number or key words or characters in the information saved with the spectra. See “Searching a library for text.”

The **Library Info** tab shows information about the library you have selected on the Library Names tab. You can also display this tab by double-clicking a library name on the Library Names tab. See “Viewing information about a library.”

The **Library Spectra** tab shows information about the spectrum you have selected on the Library Names tab. You can also display this tab by double-clicking a spectrum title on the Library Names tab. See “Viewing library spectra.”

## Working with libraries

Click the Library Names tab to display the contents of libraries and perform various operations on libraries.



There are three types of libraries:

**Search** libraries are collections of reference spectra that you can use to identify unknown spectra.

**QC** (QC Compare) libraries let you verify the quantitative 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.

**Note** The spectra in a QC library are not independent (as in a traditional search library) but instead are grouped into compound types. Because of this, the result of comparing a sample spectrum with the spectra in a QC Compare library is not a list of the best individual matches in the library but instead a list of the best match from each type. ▲

**Scrapbook** libraries are a convenient place to store and organize your spectra. You can add any spectrum to a scrapbook library; the resolution and other parameters do not matter. After adding spectra to the library, you can find them by search for text stored with the spectra. You cannot perform a spectral data search of a scrapbook library.

These types of libraries are contained in three “books” at the left side of the Library Names tab. To view the libraries contained in a book, click it. The book opens and the libraries contained in it appear as books. (If there are no libraries in a book, it does not open.)

To see the spectra in a library, click the library’s book. The book opens and the spectra in the library are listed to the right. The Index column shows the index number of each spectrum, and the Compound Name column shows the title of each spectrum. For user libraries, the Date column shows the date the spectrum was collected, and the Del column indicates, with an “X,” that a spectrum has been deleted. (Deleted spectra are cleared from the list when you compress the library.) You can click a column heading to list the spectra in the order associated with that column; for example, click the Index column heading to list the spectra in numerical order by index number. To see more of the information in the cells of a column, you can drag the vertical dividing lines between the column headings to the left or right to change the width of the column.



You can use the buttons along the top of the tab to perform the special operations listed in the following table.

To do this...	Use this button...
Create a new user library.	Create Library
Add all of the spectra in one user library to another (merge two user libraries).	Merge Library
Renumber the spectra in a user library (compress the library) to eliminate empty slots created when spectra were removed.	Compress Library
Select a library or library spectra for an operation.	Select
Place a copy of a library spectrum into a spectral window.	Add To Window
Place a copy of a user library spectrum into another user library.	Add To Library
Delete a user library spectrum from a user library.	Delete
Delete a user library.	Delete
Collect a sample spectrum and place it into a user library.	Collect Spectrum
Sign a user library.	Sign

You can print information contained on the tab with Print in the File menu.

The next sections explain how to use the buttons.

### Creating a user library



Use the Create Library button to create a user library. You can create a search library, QC library or scrapbook library. See the next section for more information about user libraries.

When you create a library, you determine the kinds of information that will be saved with it. You also set a number of parameters, including the resolution and spectral range of the library and which checks and corrections are performed.

The Library Creation Wizard leads you through the steps appropriate for the type of library you are creating. If you need further assistance, click the Help button and then the How To button in the Help window that appears. (You can also choose OMNIC Help Topics from the Help menu, find “library, creating” on the Index tab and go to the “How to create a user library” topic.)

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

**Note** You can specify a default directory for this operation in the File options (available through Options in the Edit menu). (If you have the DS option, the directory is specified by the Directory For User Libraries system policy.) ▲

### About user libraries

User libraries are intended to be used for operators of the spectrometer to create a searchable database of spectral information. The library file structure is restricted within certain parameters to ensure consistency of data within the library. To ensure your spectral libraries are consistent, it is best to use the same experiment parameter settings when collecting data that will be placed into the libraries.

If the parameter settings for spectral data collection vary because of different sampling techniques or other reasons, we recommend creating different user libraries. Keep in mind that you can search as many libraries as you desire or group multiple libraries together in OMNIC.

When you create a user library, you specify the resolution and spectral range for the library using the Library Creation Wizard. However, the resolution and spectral range values used for the library may not turn out as expected. With this in mind, note the following behavior of the library creation and subsequent additions to the library.

**Library resolution** – When the first spectrum you attempt to add to a user search library or QC library has a lower resolution (higher numerical value) than that specified when the library was created, it will not be added. A message will appear indicating that the resolution is lower than expected.

When the first spectrum you attempt to add to a user search library or QC library has a higher resolution (lower numerical value) than that specified when the library was created, it will be added. However, the spectrum will be deresolved to match the resolution of the library. No message appears in this case.

All subsequent spectra of any resolution that you attempt to add will be accepted by the library. When these spectra are added, the data point spacing (which determines the spectral resolution) is adjusted to match that of the library.

**Library spectral range** – The first spectrum you add to a user search library or QC library determines the spectral range of the library. If the spectral range specified when you created the library is different from that of the first spectrum, the library's spectral range will be adjusted.

After the first spectrum has been added and you attempt to add a spectrum with a narrower spectral range, the spectrum will not be accepted by the library. A message will appear indicating that the spectral range does not include the entire library range.

After the first spectrum has been added and you attempt to add a spectrum with a broader spectral range, the spectrum will be accepted by the library. However, the spectral range will be decreased to match the spectral range of the library. No message appears in this case.

**Collection and processing information for spectra extracted from a library** – When you extract a spectrum from a user library into a spectral window, the noneditable portion of the collection and processing information is displayed as follows:

The “Data Collection Information” section is based on the first spectrum added to the library.

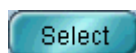
The “Data Description” section is the true description of the data in the library.

The “Spectrometer Description” section is based on the first spectrum added to the library.

The “Data Processing History” section is reset to indicate that the data was retrieved from the library.

All other information is reset to default values.

### Selecting a library or library spectra



The Select button has two functions. You can use it to select a user library that you want to merge with another user library. You can also use it to select user library spectra that you want to add to a user library.

*Follow these steps to select a library you want to merge:*

**1. Choose Library Manager from the Analyze menu.**

Library Manager appears with the Library Names tab in front.

**2. To select a user library to be merged with another user library, click the book that contains the library to be selected.**

The libraries in the book are listed.

**3. Click the name of the library you want to select.**

**4. Choose Select.**

You can now merge the selected user library with another user library. See “Merging user libraries” for details.

**Note** You can also merge libraries by dragging one user library at the left side of the Library Names tab of Library Manager onto another user library on the tab. The library you dragged is deleted after being merged with the second library. ▲

*Follow these steps to select library spectra to add to another library:*

**1. Choose Library Manager from the Analyze menu.**

Library Manager appears with the Library Names tab in front.

2. **To select one or more spectra to be added to a user library, click the library that contains the spectra.**

The spectra in the library are listed.

3. **Click the titles of the spectra you want to select.**

You can hold down the Control key to let you select more than one spectrum.

4. **Choose Select.**

You can now add the selected spectra to a user library. See “Adding user library spectra to another user library” for details.

**Note** You can also add a spectrum to a user library by dragging the spectrum or the spectrum’s file to the library’s book on the Library Names tab of Library Manager. ▲

### Merging user libraries



Use the Merge Library button to merge two user libraries. When you merge libraries, all of the spectra in the selected library are added to the current library. The resolution, zero filling and spectral range of the first library must be compatible with the second. For example, a library of 4-wavenumber resolution spectra can be merged into a 16-wavenumber library, since the 4-wavenumber spectra have a data point for each point needed by the 16-wavenumber library. On the other hand, the spectra in a 16-wavenumber library do not have the needed data points to be merged into a 4-wavenumber library.

The information in the custom text fields for the spectra in the selected library is placed in fields in the current library, with the fields kept in the same order. The field names in the current library are used, regardless of the names in the selected library.

**Notice** If there are more fields in the selected library than in the current library, the excess fields and the information contained in them are lost when you merge the libraries. Keep this in mind when you merge libraries that do not have identical fields. ▲

You can also merge libraries by dragging one user library at the left side of the Library Names tab of Library Manager onto another user library on the tab. The library you dragged is deleted after being merged with the second library.

Follow these steps to merge two user libraries:

**1. Choose Library Manager from the Analyze menu.**

Library Manager appears with the Library Names tab in front.

**2. Click the book that contains the libraries you want to merge.**

The libraries must be user libraries of the same type—search library, QC library (QC Compare) or scrapbook library—to be merged.) The libraries in the book are listed.

**3. Click the name of the user library whose spectra you want to add to another user library.**

**4. Choose Select.**

The library becomes the “selected” library.

**Notice** This library will be deleted when the libraries are merged. ▲

**5. Click the name of the user library to which you want to add the spectra.**

The library becomes the “current” library.

**6. Choose Merge.**

The spectra in the selected library are added to the current library and appear in the list of library spectra at the right. The selected library is deleted.

**7. Choose Close to close Library Manager if desired.**

**Compressing a user library**



After you delete one or more spectra from a user library, you can use the Compress Library button to remove the deleted spectra (including the "X" in the Del column) from the list of library spectra. The remaining spectra are then consecutively renumbered.

Follow these steps to compress a user library:

**1. Choose Library Manager from the Analyze menu.**

Library Manager appears with the Library Names tab in front.

**2. Click the book that contains the user library you want to compress.**

The libraries in the book are listed.

**3. Click the name of the user library you want to compress.**

**4. Choose Compress Library.**

The deleted spectra (those with an "X" in the Del column) are removed from the list, and the remaining spectra are consecutively renumbered.

**5. Choose Close to close Library Manager if desired.**

**Placing a library spectrum into a spectral window**



Click the Add To Window button to place a library spectrum into a spectral window.

**Note** There are two other ways to place a library spectrum into a spectral window:

- Double-click the spectral display pane on the Library Spectra tab. When the Add To Window dialog box appears, specify whether to add the spectrum to a new or existing window. To do this, click the arrow to the right of the window selection box and then click the desired option in the list that appears. Click the Add button to add the spectrum to the window. If you selected Add To A New Window and Prompt For New Window Title is turned on in the Window options, a dialog box asks for a title for the new spectral window. Type a title and then choose OK. (If you type the title of an existing window, a new window will be created with that title, resulting in two windows with the same title.)
- Drag the spectrum from the list of spectra at the right side of the Library Names tab of Library Manager into a pane in the window. ▲

Follow these steps to place a library spectrum into a spectral window:

**1. Choose Library Manager from the Analyze menu.**

Library Manager appears with the Library Names tab in front.

**2. Click the book that contains the library whose spectrum you want to display.**

**3. Click the name of the library.**

The spectra contained in the library are listed at the right side of the tab.

**4. Click the title of the spectrum you want to display.**

**5. Choose Add To Window.**

The Add To Window dialog box appears.



## 6. Specify whether to add the spectrum to a new or existing window.

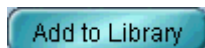
To do this, click the arrow to the right of the window selection box and then click the desired option in the list that appears.

## 7. Click the Add button to add the spectrum to the window.

If you selected Add To A New Window and Prompt For New Window Title is turned on in the Window options, a dialog box asks for a title for the new spectral window. Type a title and then choose OK. (If you type the title of an existing window, a new window will be created with that title, resulting in two windows with the same title.)

A copy of the spectrum is placed into the spectral window. You can then manipulate or process the spectrum using other OMNIC features.

### Adding user library spectra to another user library



After you select one or more user library spectra, you can use the Add To Library button to add the spectra to a user library.

**Note** The spectra in a QC library are not independent (as in a traditional search library) but instead are grouped into compound types. When you add a spectrum to a QC Compare library, you must specify which type the spectrum represents. When you later perform a QC comparison, the result is not a list of the best individual matches in the library but instead a list showing the single best match from each type. ▲

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

- Drag the spectrum from the list of spectra at the right side of the Library Names tab of Library Manager.
- Drag the spectrum from a spectral window.
- Drag the spectrum's file from Windows Explorer.

The Add To Library dialog box appears. See steps 8 through 11 in the following procedure for information on using the dialog box. ▲

Follow these steps to add user library spectra to another user library:

**1. Choose Library Manager from the Analyze menu.**

Library Manager appears with the Library Names tab in front.

**2. Click the book which contains the library that contains the spectrum you want to add.**

**3. Click the name of the library.**

The spectra contained in the library are listed at the right side of the tab.

**4. If you want to add one spectrum, click its title. If you want to add more than one spectrum, hold down the Control key and click their titles.**

**5. Choose Select.**

**6. Click the book that contains the library to which you want to add the spectra.**

**7. Click the name of the library.**

You can only add the spectra to a library that you created; you cannot add spectra to a commercial library.

**8. Choose Add To Library.**

The Add To Library dialog box shows the name of the library and the library index number that will be assigned to the spectrum.

**9. In the text boxes below Enter Field Information type the desired information for each field.**

The first field already contains the title of the spectrum. The kinds of information to be entered in the other text boxes depend on what custom information field names you specified when you created the library. The contents of these fields will be searched when you find spectra by searching for text using the Search For Text tab.

If you are adding spectra to a search library or scrapbook library, go to step 11.

**10. If you are adding the spectra to a QC library, the dialog box lets you specify whether to add the spectrum to an existing compound type or to a new type.**

To add the first spectrum to an existing type, select Add To Current Compound Type and then select one of the listed types. To add the spectrum to a new type, select Enter A Compound Type and then type a name for the new type in the text box.

**11. Choose OK to add the spectrum or OK To All to add all the selected spectra using the specifications you have made for the first spectrum.**

- If you are adding just one spectrum and chose OK, or if you are adding more than one spectrum and chose OK To All, the procedure is finished (unless a spectrum fails a specified check; this is explained below).
- If you are adding more than one spectrum and you chose OK, information for the next selected spectrum appears. Make the desired changes and then choose OK or OK To All.

If you specified that the noise level or peak intensities of added spectra be checked when you created the library, these items are checked and a message appears if a spectrum fails a check. If you want to add the spectrum to the library anyway, choose OK.

**Note** When the first spectrum you attempt to add to a user library has a lower resolution (higher numerical value) than that specified when the library was created, it will not be added. A message will appear indicating that the resolution is lower than expected. ▲

### Deleting a spectrum from a user library



Use the Delete button to delete a spectrum from a user library. (You can also use the button to delete a user library. See “Deleting a user library” for details.) Follow these steps:

**1. Choose Library Manager from the Analyze menu.**

Library Manager appears with the Library Names tab in front.

**2. Click the book that contains the user library from which you want to delete a spectrum.**

**3. Click the name of the library.**

The spectra contained in the library are listed at the right side of the tab.

**4. Click the title of the spectrum you want to delete.**

You can select more than one spectrum to delete by holding down the Control key or Shift key while clicking the titles of the spectra.

**5. Choose Delete.**

A message says the spectrum (or spectra) will be deleted.

**6. Choose OK.**

An “X” appears in the Del column in each deleted spectrum’s row, indicating that the spectrum has been deleted and is no longer available for library searches or QC comparisons. You can remove the deleted spectra from the list by using the Compress Library button.

## 7. Choose Close to close Library Manager if desired.

### Collecting a spectrum and adding it to a user library



Use the Collect Spectrum button to collect a spectrum and add it to a user library. The software automatically sets the experiment parameters (for example, Resolution) so that the spectrum will be compatible with the selected library. This lets you 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).

Follow these steps to collect a spectrum and add it to a user library:

#### 1. Choose Library Manager from the Analyze menu.

Library Manager appears with the Library Names tab in front.

#### 2. Click the book that contains the library to which you want to add the spectrum.

#### 3. Click the name of the library.

#### 4. Choose Collect Spectrum.

#### 5. Follow the instructions that appear on the screen.

#### 6. When the Add To Library dialog box appears, type the desired information for each information field.

The first field already contains the title of the spectrum. The kinds of information to be entered in the other text boxes depend on what custom information field names you specified when you created the library. The contents of these fields will be searched when you find spectra by searching for text using the Search For Text tab.

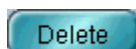
If you are collecting a spectrum to be added to a search library or scrapbook library, go to step 8.

If you are collecting a spectrum to be added to a QC library, the dialog box lets you specify whether to add the spectrum to an existing compound type or to a new type. See the next step.

- 7. To add the spectrum to an existing type, select Add To Current Compound Type and then select one of the listed types. To add the spectrum to a new type, select Enter A Compound Type and then type a name for the new type in the text box.**
- 8. Choose OK to add the spectrum.**

If you specified that the noise level or peak intensities of added spectra be checked when you created the library, these items are checked and a message appears if a spectrum fails a check. If you want to add the spectrum to the library anyway, choose OK.

### Deleting a user library



Use the Delete button to delete the selected user library from the disk. Follow these steps:

- 1. Choose Library Manager from the Analyze menu.**

Library Manager appears with the Library Names tab in front.

- 2. Click the book that contains the user library you want to delete.**
- 3. Click the name of the library.**

The spectra contained in the library are listed at the right side of the tab.

- 4. Choose Delete.**

A message asks whether to delete the library.

## 5. Choose OK. The library is deleted.

**Note** If the library file is specified in Windows as read-only, it cannot be deleted until you remove that specification. See the Windows Help system for information on changing the attributes or properties of files (search for the word “attributes” or “properties” to locate the relevant topics). ▲

## 6. Choose Close to close Library Manager if desired.

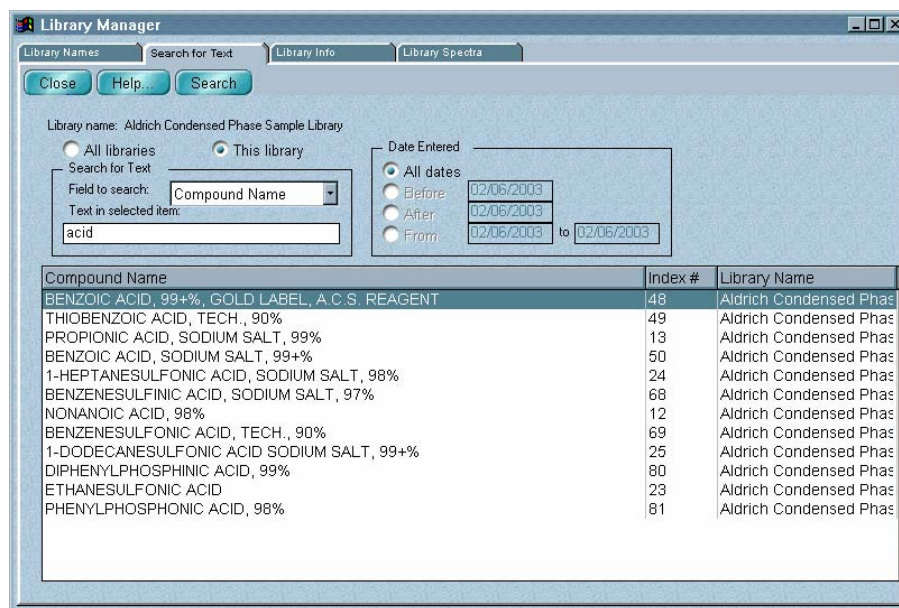
### Signing a user library



If you have the DS option, the Sign button appears on the Library Names tab allowing you to sign the selected user library. When you click the button, a prompt asks you to provide a digital signature information. After you sign the library, information about the signature appears at the bottom of Library Manager; for example, “Signature: Smith, John, 06-17-2004 12:02:37 (GMT-06:00), Authorship.” If you later change the library, the text is changed to: “Unable to verify digital signature. The data has been changed.” You may sign the library again. If you select a user library that has not been signed, “Signature: Not Signed” appears.

### Searching a library for text

Click the Search For Text tab if you want to find library spectra by searching for text in specified information fields saved with the spectra.



For example, you can search for spectra whose information contains a specific name or the date the spectrum was collected. The available fields depend on the information included with the library.

You can print information contained on the tab by using Print in the File menu.

Follow these steps to search for text:

**1. Choose Library Manager from the Analyze menu.**

Library Manager appears with the Library Names tab in front.

**2. Click the book that contains the library you want to search.**

**3. Click the name of the library.**

The spectra contained in the library are listed at the right side of the tab.

**4. Click the Search For Text tab.**

The name of the selected library is shown near the top of the tab.

**5. If you want to search only this library, select This Library. If you want to search all the libraries, select All Libraries.**

If you want to search a different library by itself, select it on the Library Names tab and then return to this tab and select This Library.

**6. Specify whether to search for text in one field or in all fields by selecting an option from the Field To Search drop-down list box.**

The available fields depend on the information included with the library. If you selected All Libraries, only the All Fields, Compound Name and Index # fields are available.



7. **Type the text to search for in the Text In Selected Item box.**
8. **To search all spectra, select All Dates. To search only spectra collected before a certain date, select Before and enter the date in the corresponding text box.**

The options in the Date Entered box let you limit the search to spectra collected during a specified time period.

Express dates on this tab in the format used by your system. For example, in the U.S.A. this is normally month/day/year, with the month and day as two-digit numbers and the year as a four-digit number. To search only spectra collected after a certain date, select After and enter the date in the text box. To search only spectra collected during a certain period, select From \_\_ To \_\_ and enter the starting and ending dates.

**Note** Libraries created using versions of OMNIC before OMNIC E.S.P. do not have date fields. Spectra in these libraries will be found only if you select the All Dates option. ▲

## 9. Choose Search.

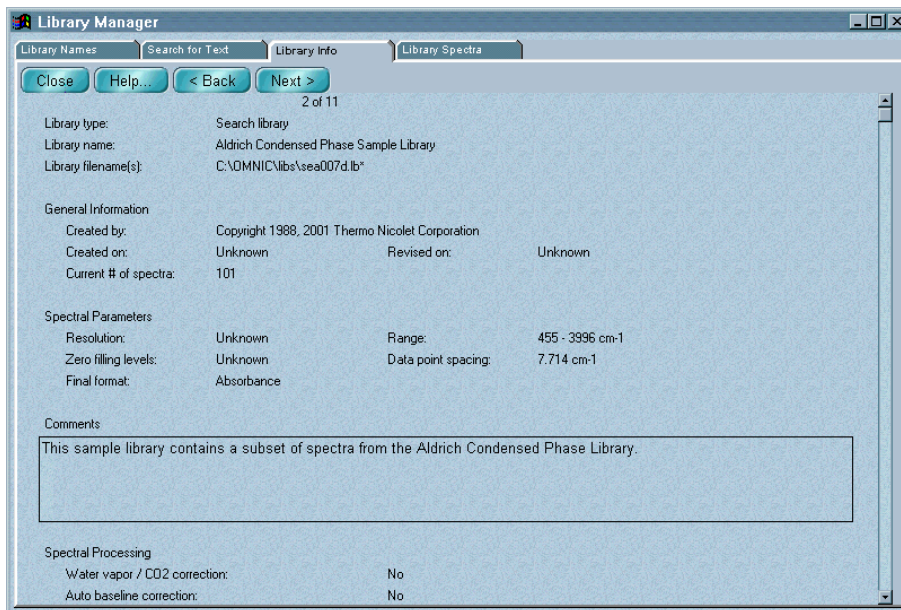
The search results appear in the table. To list the found spectra in alphabetical order by compound name, click the Compound Name column heading. To list the spectra in numerical order by index number, click the Index # heading. To list the spectra in alphabetical order by the names of the libraries that contain them, click the Library Name heading. To see more of the information in the cells of a column, you can drag the vertical dividing lines between the column headings to the left or right to change the width of the column.

To see information about a found spectrum, double-click its row in the table. The Library Spectra tab displays the information.

## 10. Choose Close to close Library Manager if desired.

## Viewing information about a library

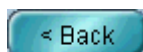
Click the Library Info tab to see the kinds of information about the selected library shown and described in the following illustration and table. You can also double-click a library name on the Library Names tab to display this information.



The number of the library is shown near the top of the tab; for example, “2 of 10” means that the selected library is the second of ten libraries in its category (search, QC Compare or scrapbook).



To see information about the next library in the category, choose Next.



To see information about the preceding library, choose Back.

Information	Description
Library Type*	The type of library: search library, QC library (QC Compare) or scrapbook library.
Library Name*	The name of the library.
Library Filename(s)	The pathnames of the files that contain the library spectra.
Created By*	The person who created the library.
Created On*	When the library was created.

Information	Description
Revised On	When the library was last changed.
Current # Of Spectra	The number of spectra in the library.
Resolution*	The spectral resolution of the library spectra.
Range*	The spectral range of the library spectra.
Zero Filling Levels*	The number of levels of zero filling.
Data Point Spacing	The data spacing of the library spectra.
Final Format*	The Y-axis format of the library spectra.
Comments*	Any comments stored with the library. You can change the comments for a user library by editing the text in the Comments text box.
Water Vapor/CO2 Correction**	Whether the library spectra were corrected for water and carbon dioxide.
Auto Baseline Correction**	Whether the baseline of the library spectra were corrected automatically.
Signal-To-Noise Check**	Whether the signal-to-noise ratios of the library spectra were checked.
Band Intensity Check**	Whether the library spectra were checked for totally absorbing bands.
Library Fields	A list of the custom information fields in the library.
Auto Calculate Threshold***	Shows whether the comparison threshold is calculated automatically. You can change this specification by turning the check box on or off. If the check box is on, the Current Threshold value is not used.
Current Threshold***	Shows the comparison threshold used if Auto Calculate Threshold is off. You can change this specification by typing a different value in the text box.

\* For user libraries you enter the information for these items when you create the library.

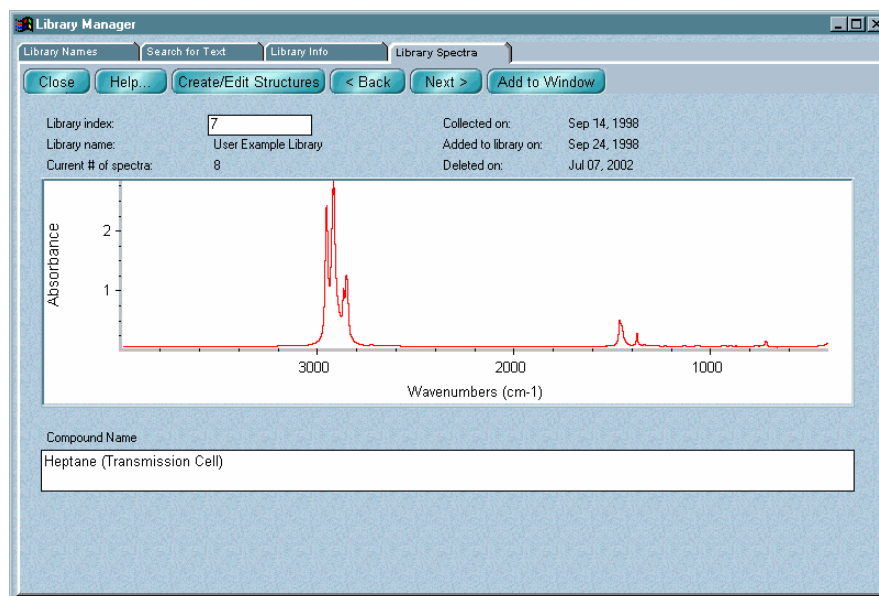
\*\* For user libraries you specify these corrections and checks when you create the library.

\*\*\* These items are displayed only for QC libraries.

You can print information contained on the tab by using Print in the File menu.

## Viewing library spectra

After you select a library (or a spectrum in a library) on the Library Names tab, click the Library Spectra tab to see information about spectra in the library. You can also double-click a spectrum title on the Library Names tab to display this information.



The kinds of information displayed will vary depending on whether you selected a commercial library or a library you set up using the Create Library button in Library Manager. The information described in the following table is normally shown for any library spectrum.

Information	Description
Library Index	The index number of the spectrum. Each spectrum is assigned a sequential index number when you add it to a library.
Library Name	The name of the library that contains the spectrum.
Current # Of Spectra	The number of non-deleted spectra in the library.
Collected On	When the spectrum was collected.

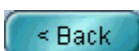
Information	Description
Added To Library On	When the spectrum was added to the user library.
Deleted On	When the spectrum was deleted from the user library.
Spectral Display	An image of the spectrum.
Compound Type*	The compound type you specified when you added the spectrum to the library.
Compound Name	The name of the compound.

\* This information is displayed only for spectra in QC libraries.

You can edit the text in a custom information field of a user library directly. When you display another library spectrum or a different tab, you are asked whether to save your changes. Respond as desired to the prompt.

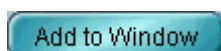


To see information about the next spectrum in the library, choose Next.



To see information about the preceding spectrum, choose Back.

If you know the index number of a spectrum, you can display it by typing its number in the Library Index text box and then pressing Enter.



You can place a library spectrum into a spectral window by double-clicking the spectral display pane on the Library Spectra tab or by clicking the Add To Window button near the top of the tab. When the Add To Window dialog box appears, specify whether to add the spectrum to a new or existing window. To do this, click the arrow to the right of the window selection box and then click the desired option in the list that appears. Click the Add button to add the spectrum to the window. If you selected Add To A New Window and Prompt For New Window Title is turned on in the Window options, a dialog box asks for a title for the new spectral window. Type a title and then choose OK. (If you type the title of an existing window, a new window will be created with that title, resulting in two windows with the same title.)

If you have the optional ACD/ChemSketch<sup>®</sup> DB software, you can use the Create/Edit Structures button to draw chemical structures. See the next section for details.

You can print information contained on the tab by using Print in the File menu.

### Drawing or editing chemical structures

Create/Edit Structures

If you have the optional ACD/ChemSketch<sup>®</sup> DB software, you can use the Create/Edit Structures button to draw chemical structures and save them with the spectra in a user library. When you later view the spectra on this tab, the structure for each spectrum is displayed in a small window. Also, if a library spectrum with a saved structure is found when you search the library, you can display the structure by selecting the spectrum in the list of matches.

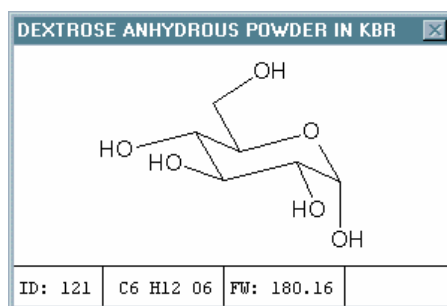
Follow these steps:

1. **On the Library Spectra tab of Library Manager, display a user library spectrum for which you want to draw or edit a chemical structure.**

You can display a spectrum by selecting it on the Library Names tab and then clicking the Library Spectra tab or by using the Back and Next buttons on the Library Spectra tab to browse through the spectra.)

If you have already drawn a structure for any spectrum in the library, a window shows the structure for the spectrum, if one exists.

Here is an example:



**2. Click the Create/Edit Structures button near the top of the tab.**

The ACD/ChemSketch DB software starts.

**3. Draw or edit the structure for the spectrum.**

See the documentation that came with the ACD/ChemSketch DB software for complete information.

**4. Click the OK button at the bottom of the ACD/ChemSketch DB window.**

Do *not* choose Exit or Save from the File menu. The structure appears in a smaller window that you can position as desired. The window title shows the name of the compound. The index number (ID) of the spectrum and the chemical formula and molecular weight (MW) of the compound (based on the drawn structure) appear at the bottom of the window.

**5. Repeat steps 1 through 4 for the next spectrum for which you want to draw or edit a structure.**

You can click the Back or Next button on the Library Spectra tab to move through the spectra in the library and draw or edit structures for as many spectra as you wish.

The window that displays the structures is closed when you display another tab or close Library Manager.

**Note** If a library spectrum with a saved structure is found when you search the library, you can display the structure by selecting the spectrum in the list of matches. You can also print the structure by using the Print button in the Search window. ▲

## — **How to** ➔ Manage libraries

### 1. **Choose Library Manager from the Analyze menu.**

Library Manager appears with the Library Names tab in front.

### 2. **Display the tab that contains the features you want to use by clicking the tab.**

- The Library Names tab lets you view the contents of libraries and perform the following operations:

Create a new user library. See “Creating a user library.”

Add all of the spectra in one user library to another (merge two user libraries). See “Merging user libraries.”

Renumber the spectra in a user library (compress the library) to eliminate empty slots created when spectra were removed. See “Compressing a user library.”

Place a copy of a library spectrum into a spectral window. See “Placing a library spectrum into a spectral window.”

Select a library or library spectra for an operation. See “Selecting a library or library spectra.”

Place a copy of a spectrum into a user library. See “Adding user library spectra into another user library.”

Delete a library spectrum from a user library. See “Deleting a spectrum from a user library.”

Delete a user library. See “Deleting a user library.”

Collect a sample spectrum and place it into a user library. See “Collecting a spectrum and adding it to a user library.”

- The Search For Text tab lets you find library spectra by searching for text saved with the spectra. See “Searching a library for text.”



- The Library Info tab lets you view detailed information about libraries. See “Viewing information about a library.”
- The Library Spectra tab lets you view detailed information about spectra in libraries. See “Viewing library spectra.”

**3. To print the information contained on the tab, choose Print from the File menu.**

The Print dialog box appears. The options available in the dialog box depend on which tab you are using.

If you want to print the list of libraries, turn on List Of Libraries.

If you want to print the list of library spectra, turn on List Of Library Spectra.

If you want to print the information about the current library, turn on Library Information.

If you want to print the information about the current library spectrum, turn on Library Spectra Information.

If you want each item printed on a separate page, turn on Print Items On Separate Pages.

To set up the printer, choose Printer Setup. The Print Setup dialog box appears. Select the printer from the list box. You can also specify portrait or landscape page orientation.

**Note** If you change the orientation, the Orientation option in the Print options (available through Options in the Edit menu) will be reset to the new orientation. The page orientation setting in Windows Control Panel or in the printer setup dialog box for other applications is not affected by the setting you make here. ▲

If you want to set the printer parameters, choose Properties in the Print Setup dialog box. If you don't want to set the parameters, choose OK. If you choose Properties, a dialog box shows the current settings of the printer parameters. This dialog box varies in appearance depending on your printer. See the documentation that came with your printer for information on setting the printer parameters. After you set the parameters, choose OK to close the dialog box, and then choose OK to close the Print Setup dialog box.

When you are ready to start printing, choose OK.

**4. When you are finished using Library Manager, choose Close.**

## Setting up a QCheck comparison

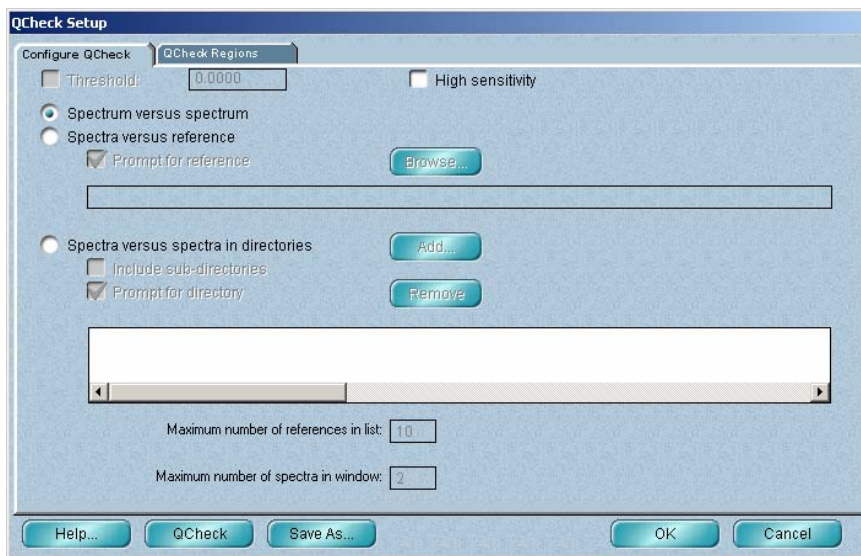
The QCheck Setup parameters are a subset of the Search parameter group contained in the current experiment file. You can save your parameter settings by using the Save As button in the QCheck Setup dialog box or by saving the experiment using Experiment Setup in the Collect menu.

**How to** ➔

Set up a QCheck comparison

**1. Choose QCheck Setup from the Analyze menu.**

The QCheck Setup dialog box appears:



## 2. Set the parameters on the Configure QCheck tab.

Select High Sensitivity if you want the results displayed using an expanded Y scale that makes it easier to see differences between very similar spectra.

Select the type of comparison to perform:

**Spectrum Versus Spectrum** compares two selected spectra. If you select this type, skip to step 4.

**Spectra Versus Reference** compares one or more selected spectra with a reference spectrum (or spectral group).

- To specify that spectrum (or group) now, deselect Prompt For Reference and use the dialog box that appears. The path to the specified spectrum appears below the Browse button. You can use that button to change the specification.
- To be prompted for the reference during the comparison procedure, leave Prompt For Reference selected (or select it if it is not selected).

**Spectra Versus Spectra In Directories** compares one or more selected spectra with the spectra in one or more directories.

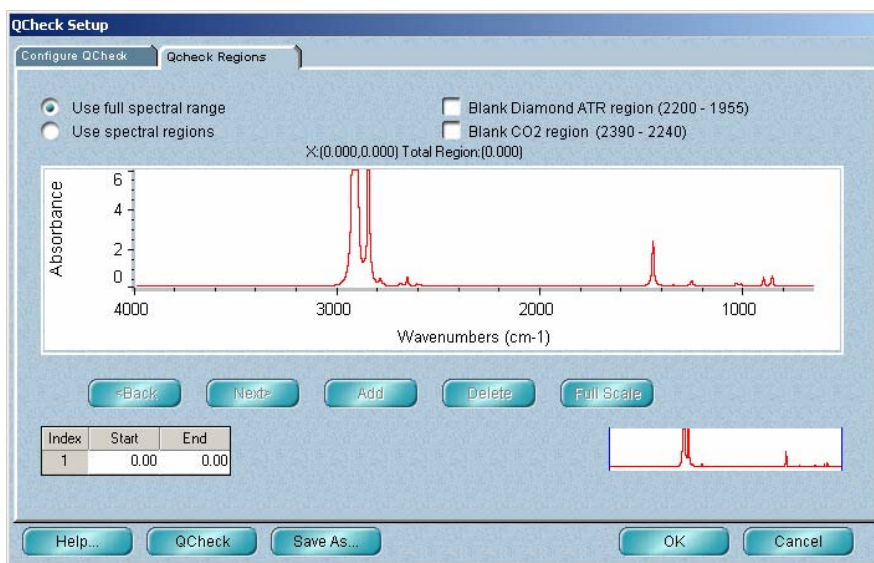
- To specify those directories now, deselect Prompt For Directory and use the dialog box that appears to specify a directory. The path to the specified directory appears in the list box. You can add another directory to the list by using the Add button. You can remove a directory from the list by selecting the directory and choosing Remove. To include spectra in sub-directories in the comparison, select Include Sub-directories.

Additional parameters are available for the latter two comparison types:

- To use a “pass/fail” threshold for the comparison, select Threshold and enter the desired minimum correlation value in the text box. A value of 1.0 is the highest allowed setting and indicates a perfect match. In the results, spectra whose QCheck correlation value is equal to or greater than the entered value will “pass” the comparison; spectra whose correlation value is less will “fail.”

- Set Maximum Number Of References In List to the maximum number of spectra to include in the results. (This parameter is available for Spectra Versus Reference only if the reference is a spectral group.)
- Set Maximum Number Of Spectra In Window to the maximum number of spectra to display. (This parameter is available for Spectra Versus Reference only if the reference is a spectral group.)

### 3. Specify the spectral regions to use in the comparison by setting the parameters on the QCheck Regions tab.



- To include the full spectral range of data, select **Use Full Spectral Range**.
- To specify the spectral regions to include, select **Use Spectral Regions**. To make it easier to specify regions, you can use the view finder to expand the data display and choose Full Scale to display the data full scale.

To specify the region graphically, drag across the region in the spectral display pane. The region is shaded and bordered by vertical lines. The limits of the region appear above the pane and in the table in the lower-left corner of the tab. You can change the limits by dragging the triangular handles.

To specify the region using the table, click the cell below Start and type the starting limit. Then click the cell below End and type the ending limit. You can press Enter to enter a value you typed.

After you have specified a region, choose Add. The Index number in the table increases by one, and you can specify the next region using the same techniques. You can view the regions you have specified by using the Back and Next buttons.

**Note** If you do not specify any regions for the Use Spectral Regions option, QCheck will use the intersection of the spectral ranges of the spectra being compared. ▲

To exclude data in the region from 2200 wavenumbers to 1955 wavenumbers (where diamond ATR crystals absorb radiation), select Blank Diamond ATR Region.

To exclude data in the region from 2390 wavenumbers to 2240 wavenumbers (where carbon dioxide absorbs radiation), select Blank CO<sub>2</sub> Region.

**4. Choose OK to close the dialog box, or choose QCheck to start the QCheck comparison immediately.**

If you choose OK, you can start a comparison by choosing QCheck from the Analyze menu. Choose Cancel if you don't want your parameter settings saved.

**Note** To save your settings in an experiment file, use the Save As button. Be sure to select the Search parameter group in the Save Experiment As dialog box. Each time you open the saved experiment, the parameters will be set automatically. ▲

## Comparing spectra with QCheck

After you have set up a QCheck comparison with QCheck Setup in the Analyze menu, use QCheck in the Analyze menu to compare spectra to determine their degree of similarity, expressed as a correlation value from 0.0 (no similarity) to 1.0 (the spectra are identical).

You can compare spectra in any of the following ways:

- Compare two selected spectra.
- Compare one or more selected spectra with a reference spectrum (or spectral group).
- Compare one or more selected spectra with the spectra in one or more directories.

A correlation algorithm is used for the comparison. It removes any effect of offset in the spectra and reduces the effects of baseline variation.

When the QCheck comparison results are displayed, you can view the spectra, their correlation values and information about the spectra. You can also copy and print the results.

**Note** QCheck can be used only with spectral data files that have the extension .spa or .spg. ▲

### ■ *How to* ➔

Compare spectra with QCheck

1. **Use QCheck Setup in the Analyze menu to set up the comparison.**
2. **If Spectrum Versus Spectrum was selected in the QCheck Setup dialog box, select the two spectra to compare. If Spectra Versus Reference or Spectra Versus Spectra In Directories was selected instead, select all the spectra you want compared with the reference spectrum (or spectral group) or directory of spectra.**
3. **Choose QCheck from the Analyze menu.**

If you are comparing spectra with a reference spectrum (or spectral group) that has not yet been specified, the Select Reference dialog box appears. Locate and select the desired file and then choose Open.

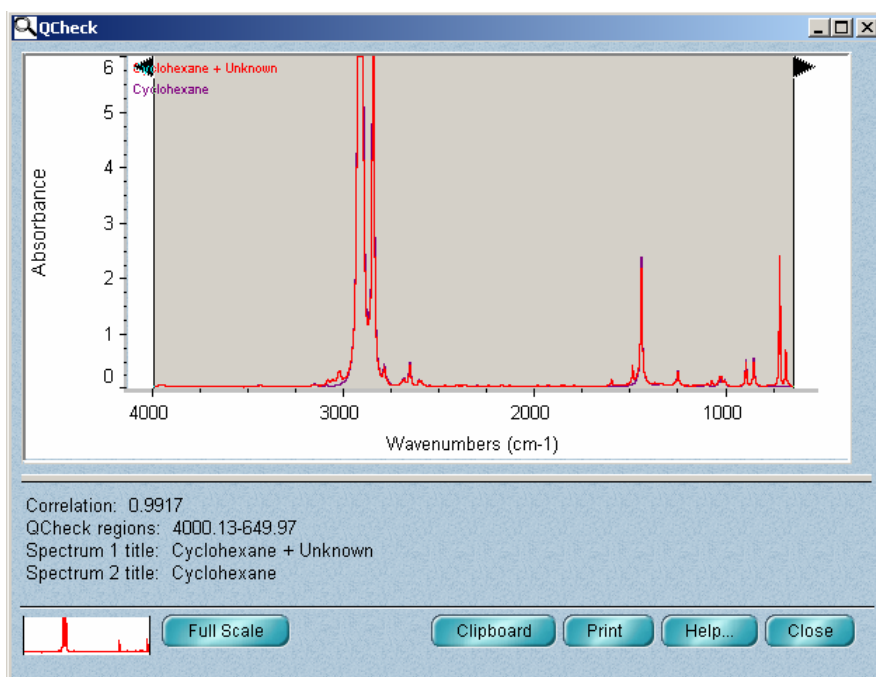
If you are comparing spectra with a directory of spectra that has not yet been specified, the Select Reference Directory dialog box appears. Locate and select the desired directory and then choose Select.\

The QCheck window appears.

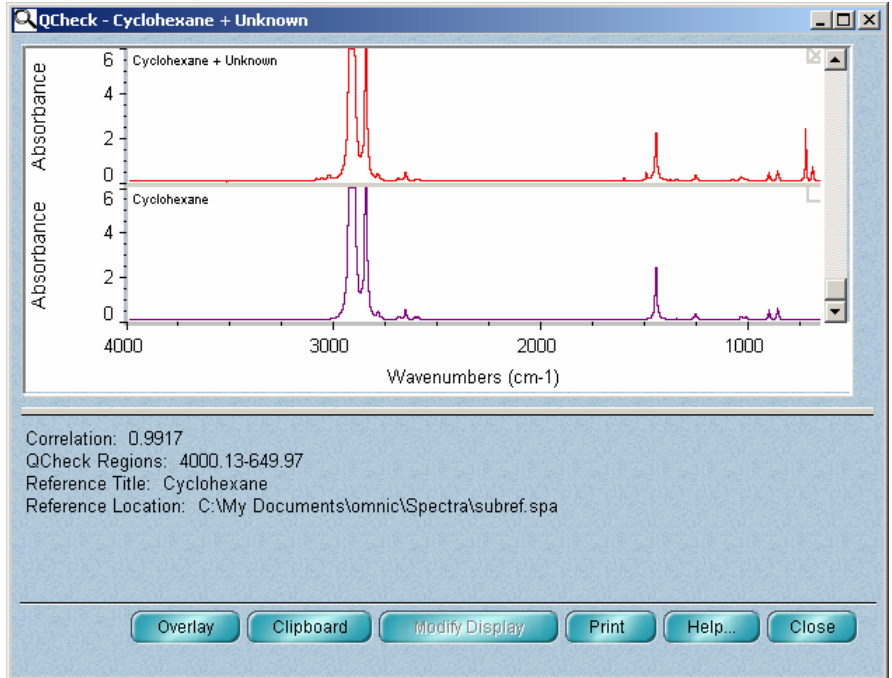
**Note** If Spectra Versus Reference or Spectra Versus Spectra In Directories was selected in the QCheck Setup dialog box and multiple spectra were selected in the spectral window, a comparison is performed on each selected spectrum and the results are displayed in separate QCheck windows. ▲

The appearance of the window varies depending on the QCheck Setup settings and the number of spectra being compared. Here are some examples:

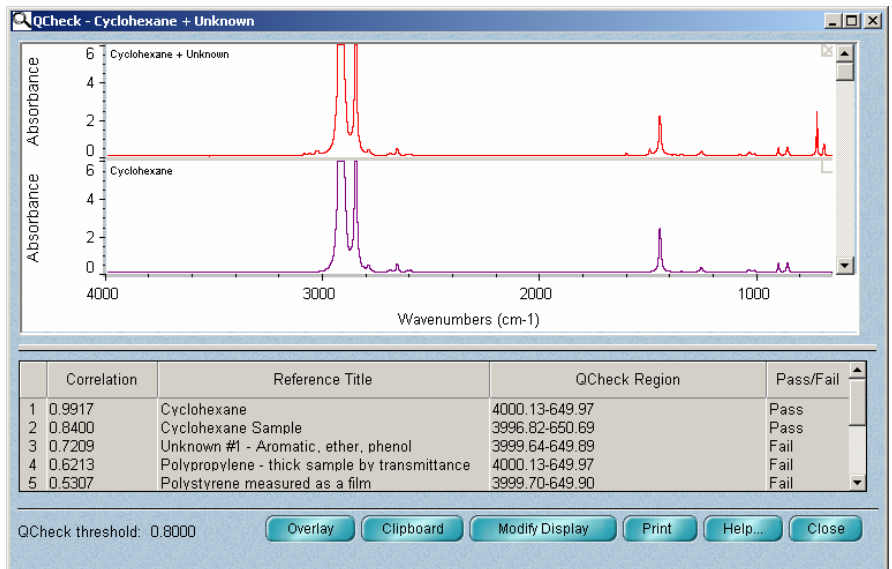
The Spectrum Versus Spectrum option was selected for this example.



The Spectra Versus Reference option was selected for this example, which compares the original spectrum with a single reference.



The Spectra Versus Spectra In Directories option was selected for this example, which uses a correlation threshold of 0.8000. Notice the results in the Pass/Fail column.

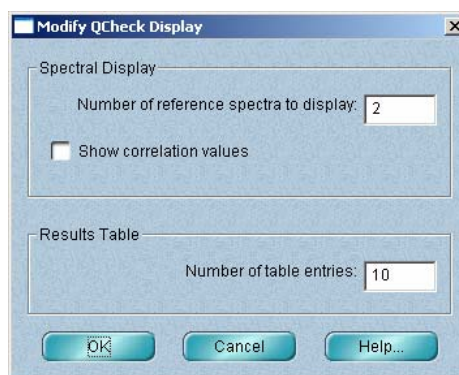


- If Spectrum Versus Spectrum was selected in the QCheck Setup dialog box, the two selected spectra are overlaid in the spectral display, and the comparison results appear below. The displayed correlation value is for the indicated spectral region. To see the results for a different region, drag the triangular handles within the pane to change the region limits. You can use the view finder in the lower-left corner of the window to zoom in on a region or expand the spectrum. To display the data full scale, choose Full Scale.



- If Spectra Versus Reference was selected, the original selected spectrum and the reference spectrum are stacked in the spectral display, and the comparison results appear below.

If the specified reference is a spectral group, the reference spectra are stacked in a scrollable spectral display and the comparison results appear in a scrollable table. To change the number of displayed spectra or the number of spectra listed in the table, choose Modify Display and set the parameters in the Modify QCheck Display dialog box:



Select Show Correlation Values if you want the correlation values of displayed spectra to appear in their panes. Choose OK when you are finished.

- If Spectra Versus Spectra In Directories was selected, the original selected spectrum and the spectra in the specified directories are stacked in the scrollable spectral display, and the comparison results appear below.

If the specified directories contain multiple spectra, the results appear in a scrollable table. Use the Modify Display button as explained above to change the number of displayed or listed spectra and to specify whether to display correlation values in the spectral display.

If you selected Threshold in the QCheck Setup dialog box, the threshold value appears in the lower-left corner of the window. You can drag the horizontal bar below the spectral display to allocate more or less space to the display.

If the displayed spectra are stacked, choose **Overlay** to overlay them; choose **Stack** to return to the stacked display.

To copy the results to the Windows Clipboard, choose **Clipboard**. You can then paste the results into a program that can accept items from the Clipboard.

To print the results, choose **Print**. In the Print dialog box select the items to print. If you print result details, signature lines will be included. If **Print Items On Separate Pages** is available, use it to specify whether to print the spectra and result details on separate pages. To set up the printer, use the **Printer Setup** button (see the Note below). Choose **OK** in the Print dialog box to print the selected items.

**Note** If you change the orientation in the Print Setup dialog box, the Orientation option in the Print options (available through **Options** in the Edit menu) will be reset to the new orientation. The page orientation setting in Windows Control Panel or in the printer setup dialog box for other applications is not affected by the setting you make here. ▲

#### 5. Choose **Close** to close the QCheck window.

## Viewing a library

If you have added **View Library** to the Analyze menu using **Edit Menu** in the Edit menu, you can use the command to view the contents of a library, see information about a library or delete a spectrum from a user library.

### — *How to* ➔

View a library

#### 1. Choose **View Library** from the Analyze menu.

The Select Library dialog box lists the libraries available on the hard disk. The libraries are listed by their library names, not by their filenames.

**2. From this dialog box you can open a library to view its contents, see information about a library or delete a spectrum from a user library.**

- To open a library, select the library name from the list in the Open Library box and then choose OK. A dialog box lists the compounds in the library in alphabetical order.

The name of the library you opened appears in the title bar of the dialog box. You can add the spectrum of a compound to a spectral window by selecting the spectrum in the list, selecting the desired option from the window selection box and choosing Add.



To delete a spectrum from a user library, select the spectrum in the list and then choose Delete. A message says that the spectrum will be deleted. Choose OK.



To print a list of the library spectra, choose Print. The Print dialog box appears.

Make sure the List Of Library Spectra check box is turned on.

**Note** The Print Items On Separate Pages option does not affect the printing of the list of spectra. ▲

To set up the printer, choose Printer Setup. The Print Setup dialog box appears. Select the printer from the list box. You can also specify portrait or landscape page orientation.

**Note** If you change the orientation, the Orientation option in the Print options (available through Options in the Edit menu) will be reset to the new orientation. The page orientation setting in Windows Control Panel or in the printer setup dialog box for other applications is not affected by the setting you make here. ▲

To set the printer parameters, choose Properties in the Print Setup dialog box. If you don't want to set the parameters, choose OK. If you choose Properties, a dialog box shows the current settings of the printer parameters. This dialog box varies in appearance depending on your printer. See the documentation that came with your printer for information on setting the printer parameters. After you set the parameters, choose OK to close the dialog box, and then choose OK to close the Print Setup dialog box.

When you are ready to start printing, choose OK.



To see information about a spectrum in the library, select the spectrum in the list box and then choose Info. The Spectrum Information dialog box appears.

When you are finished viewing the information, choose Close.

When you are finished viewing the contents of the library, choose Close to exit the View Library command.

- To see information about a library, select the library name from the list in the Open Library box and then choose Info. The Library Information dialog box appears.

To see information about a library, select the library name from the list in the Open Library box and then choose Info. The Library Information dialog box appears. The information in this dialog box generally includes the name of the library, the number of spectra the library contains, the data spacing of the spectra, etc. The kinds of information included varies depending on whether you selected a commercial library or a library you set up using the Create Library in Library Manager.

When you are finished viewing the information, choose Close to return to the Select Library dialog box. You can then see information about another library or open a library to view its contents. To close the View Library dialog box, choose Close.

## Creating a user library

If you have added Create Library to the Analyze menu using Edit Menu in the Edit menu, you can use the command 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. If you need help using the wizard, click the Help button and then the How To button in the Help window that appears. Although the procedures in Help explain how to use the wizard when it is displayed by the Create Library button in Library Manager, the steps are the same starting with step 2.

## Adding spectra to a user library

Use Add To Library in the Analyze menu to add spectra to a user library. When you add a spectrum, you also enter descriptive information into up to five fields. (The number depends on how many fields were specified when the library was created.) You can view this information during or after a library search or QC comparison.

**Note** You can also add a spectrum to a user library by dragging the spectrum from a spectral window or the list of spectra at the right side of the Library Names tab of Library Manager to the library's book on the Library Names tab. The Add To Library dialog box appears. See the procedure later in this section for information on using the dialog box. ▲

**Note** The spectra in a QC library are not independent (as in a search library) but instead are grouped into compound types. When you add a spectrum to a QC Compare library, you must specify which type the spectrum represents. When you later perform a QC comparison, the result is not a list of the best individual matches in the library but instead a list showing the single best match from each type. ▲

### — How to ➡

Add spectra to a user library

#### 1. Select the spectra.

**2. Choose Add To Library from the Analyze menu.**

The Select Library dialog box lists all the user libraries available in the currently specified library directories of the hard disk. (These are the directories listed in the Library Directories list box on the Library Directories tab of the Library Setup dialog box.) You can only add the spectrum to a library that you created; you cannot add a spectrum to a commercial library.

**3. Select the user library you want to add the spectrum to from the list.**

**Note** If you want to see information about a library before selecting it, select the library name and then choose Info. A dialog box will appear displaying information about the library. When you are finished reading the information, choose Cancel to return to the Select Library dialog box. ▲

**4. Choose OK.**

The Add To Library dialog box shows the name of the library and the library index number that will be assigned to the spectrum.

**5. In the text boxes below Enter Field Information type the desired information for each field.**

The first field already contains the title of the spectrum.

The kinds of information to be entered in the other text boxes depend on what custom information field names you specified when you created the library. The contents of these fields will be searched when you find spectra by searching for text using the Search For Text tab.

If you are adding spectra to a search library or scrapbook, go to step 7.

If you are adding the spectra to a QC library, the dialog box lets you specify whether to add the spectrum to an existing compound type or to a new type. See the next step.

6. **To add the first spectrum to an existing type, select Add To Current Compound Type and then select one of the listed types. To add the spectrum to a new type, select Enter A Compound Type and then type a name for the new type in the text box.**
7. **Choose OK to add the spectrum or OK To All to add all the selected spectra using the specifications you have made for the first spectrum.**
  - If you are adding just one spectrum and chose OK, or if you are adding more than one spectrum and chose OK To All, the procedure is finished (unless a spectrum fails a specified check; this is explained below).
  - If you are adding more than one spectrum and you chose OK, information for the next selected spectrum appears. Make the desired changes and then choose OK or OK To All.

If you specified that the noise level or peak intensities of added spectra be checked when you created the library, these items are checked and a message appears if a spectrum fails a check. If you want to add the spectrum to the library anyway, choose OK.

## Selecting a quant method

Use Quant Setup in the Analyze menu to select the quantitative analysis method you want to use to quantify a spectrum (see “Quantifying a spectrum” for details). The method must be calibrated using an optional OMNIC quantitative analysis software package. See the documentation that came with that software for information on calibrating quantitative analysis methods.

### — How to ➡

Select a quant method

#### 1. Choose Quant Setup from the Analyze menu.

The Open Quant Method dialog box lists all the quantitative analysis methods available in the directory specified in the File options (available through Options in the Edit menu).

**Note** If you have the QuantPad software, the Quant Setup dialog box appears when you choose Quant Setup. Choose Select Method in the dialog box to display the Open Method dialog box. ▲

**2. Locate the desired method and select it by clicking its filename.**

Method files have the extension .QNT.

**Note for DS systems**

If Prevent Changing Directories When Opening Files is selected in the system policies, you cannot change directories or drives to locate a method to select. ▲

When you select a method file, the title of the quantitative analysis method appears in the Quant Method Title box. The quantitative analysis software that was used to create the method is identified in the Origin box. Make a note of this information. It will be useful if you need to find documentation to help you interpret analysis results obtained with the method.

**3. If you want to reset the data collection and spectrometer parameters to match the method you are opening, turn on the Collect and Bench check boxes.**

Resetting the parameters here is a convenient way to prepare for collecting sample spectra to be analyzed with the method. This eliminates the need to use Experiment Setup to set the parameters.

**4. Choose OK.**

If you selected a method developed using PLSplus/IQ™ software, a message asks you to specify a subcalibration. Select a subcalibration from the drop-down list box and then choose OK. See the documentation that came with your PLSplus/IQ software for information on developing methods with it.

## Quantifying a spectrum

Use Quantify in the Analyze menu to find the concentrations of components in a sample spectrum. The quantitative analysis method you have selected using Quant Setup will be used for the analysis (see “Selecting a quant method” for details). The method must be calibrated using an optional OMNIC quantitative analysis software package. See the documentation that came with that software for information on calibrating quantitative analysis methods.



**— How to ➡** Quantify a sample spectrum

- 1. Select the sample spectrum.**
- 2. Use Quant Setup in the Analyze menu to select a quant method.**
- 3. Choose Quantify from the Analyze menu.**

Depending on the quant method you are using, you may be prompted to enter needed information. Follow the instructions that appear on the screen.

When the analysis is finished, a dialog box shows the results. The results may indicate the concentration of a component or provide other kinds of information, such as peak height or match value. See the documentation that came with the quantitative analysis software for complete information on interpreting the analysis results.

**Note** The name of the quantitative analysis software used to develop the analysis method was shown in the Origin box when you set up the analysis using Quant Setup. ▲

If a problem occurred during the analysis, a warning may appear in the dialog box. See the documentation that came with your quantitative analysis software for instructions on interpreting warnings.

- 4. Choose OK to close the dialog box.**



# Report

The Report menu includes commands that let you create and use report templates to arrange spectra and other items that you want to print on paper or store in on-line notebooks:

To do this...	Use this command...
Select a report template for printing reports or adding reports to a notebook, edit a template or create a new template.	Template
View a report as it would appear on paper and print it.	Preview/Print Report
Create a new report notebook to which you can add reports.	New Notebook
Add a report to a report notebook.	Add To Notebook
View a report notebook.	View Notebook

For an overview of how to use these commands, see the next section. Detailed instructions for using individual commands are provided later in this chapter.

## Working with reports

OMNIC's report and report notebook features let you create, print and save reports that contain the results of your work in formats that you select or design. Saving your work as reports in a notebook lets you easily find information later and print it out using a consistent format. OMNIC includes several example report templates suitable for laying out a variety of information. You can also create your own templates tailored to showing the kinds of information you work with.

The report templates provided with OMNIC are in the C:\My Documents\OMNIC\Report directory (or other location where you installed OMNIC). To use one of these templates to create a report, use Template in the Report menu. You can also use the Template command to edit a template or create a new template. See "Selecting, editing or creating a report template" for details.

To view or print a finished report, use Preview/Print Report in the Report menu. See “Previewing or printing a report” for details.

You can save your reports in notebooks you create. These notebooks are much like the laboratory notebooks you may have used to record your work. To view the contents of a notebook, use View Notebook in the Report menu (see “Viewing and using report notebooks”). To add a report to a notebook, use Add To Notebook in the Report menu (see “Adding a report to a notebook”). To create a notebook, use New Notebook in the Report menu (see “Creating a new report notebook”).

Follow these general steps to create, print and save a report:

- 1. If you are creating a new report template, set Margins and Orientation in the Print options (available through Options in the Edit menu) to the way you want reports printed with the template to appear.**

See “Setting the Print options for printing reports” for details.

- 2. Use Template in the Report menu to select, edit or create a report template.**

You can see a “preview” image of any existing template by selecting the template in the dialog box that appears when you choose Template.

- If you choose to edit or create a template, it is displayed in the Report Template window. Go to the next step.
- If you just select a template, it is not displayed in a window. The template will be filled in with the appropriate information when you use it to print a report. Go to step 5.

- 3. Use the features in the Report Template window to create or edit the template.**

Save your changes by using the Save As button. Close the Report Template window by clicking the Close button.

**4. Use Template in the Report menu to select the template.**

See “Selecting, editing or creating a report template” for details.

**5. Use the Print options (available through Options in the Edit menu) to set the parameters that control how the report will be printed.**

**6. Perform the operations whose results you want included in the report.**

For example, if the template you are using includes library search results, perform a library search. If the template includes a spectral window, display the desired spectrum in the spectral window. This information will appear in the report when you preview it or print it in the next step.

**7. Preview and print the report by using Preview/Print Report in the Report menu.**

See “Previewing or printing a report” for details.

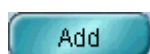
**8. If desired, add the report to a notebook by using Add To Notebook in the Report menu.**

See “Adding a report to a notebook” for details.

You can later view and print the report from within the notebook by using View Notebook in the Report menu. See “Viewing and using report notebooks.”

The use of the features in Report Template window is explained in detail in the next sections.

## **Adding an item to a report template**



Use the Add button in the Report Item box to add an item to a report template you are creating or editing.

You can add the item types described in the following table.

Type	Description
Spectral Window	<p>An image of the spectral display of the spectral window specified in the Link This Item To box. If Link This Item To is set to Active Spectral Window, and a Search window containing displayed spectra is active, the image will be the spectral display of the Search window.</p> <p>If you want just certain spectra in the window to appear in a report, be sure to display only those spectra. You can use Hide Spectra in the View menu to hide the other spectra.</p>
Text	<p>Text that you can edit directly in the Report Template window. The initial text that appears in the window is "Default Text." Use standard editing techniques to change the text as desired.</p>
Prompt For Text	<p>If you select this type, you will be prompted to enter the desired text when you preview or print a report. When prompted, type the text in the text box and choose OK. The text you enter will appear on paper at the specified location.</p>
Clipboard Picture	<p>The contents of the Windows Clipboard at the time the template was created. The contents must be in bitmap or Windows metafile format. Use this feature to add to a report an image you have copied onto the Clipboard using another program. This is most useful when you want your reports to include an image that doesn't change; for example, a corporate logo or chemical structure.</p>
Current Clipboard Picture	<p>The contents of the Clipboard at the time you preview the report before printing it. The contents must be in bitmap or Windows metafile format. This item is useful when you want to generate reports for a variety of samples, each report having the same layout but containing a unique image such as a video image of the sample captured using <math>\mu</math>View<sup>™</sup> or OMNIC Atlus<sup>™</sup>.</p>
Date And Time	<p>The current date and time.</p>

Type	Description
Spectrum Title	The title of the selected spectrum in the linked spectral window (specified in the Link This Item To box). If more than one spectrum is selected, the title of the spectrum that was selected first is used.
Spectrum Comments	The comments for the selected spectrum in the linked spectral window (specified in the Link This Item To box). These are the same comments as are displayed in the Collecting And Processing Information window for the spectrum.
Spectrum Custom Info 1	The text contained in the Custom Info 1 text box in the Collection And Processing Information window for the spectrum.
Spectrum Custom Info 2	The text contained in the Custom Info 2 text box in the Collection And Processing Information window for the spectrum.
Spectral Quality	The spectral quality information for the selected spectrum in the linked spectral window (specified in the Link This Item To box). This includes the results of any quality checks performed when the spectrum was collected.
Spectrum History	The data processing history of the selected spectrum in the linked spectral window (specified in the Link This Item To box).
Collection Time	The date and time the selected spectrum in the linked spectral window (specified in the Link This Item To box) was collected. If more than one spectrum is selected, the collection time of the spectrum that was selected first is used.
Collection Information	The data collection information for a spectrum in a linked spectral window. This includes the number of sample and background scans and the resolution, gain, optical velocity and aperture values.

Type	Description
Bench Configuration	The spectrometer configuration information for the selected spectrum in the linked spectral window (specified in the Link This Item To box). This includes the detector, beamsplitter and source. If more than one spectrum is selected, the information for the spectrum that was selected first is used.
Search Result	The spectral search results for the selected spectrum in the linked spectral window (specified in the Link This Item To box). This information is identical to the search results that appear in the log window. Search results will appear in the report only if the spectrum was the last to be searched.
QC Comparison Result	The results of the last QC comparison. This information is identical to the comparison results that appear in the log window.
Quant Result	The quantitative analysis results obtained using the Quantify command for the selected spectrum in the linked spectral window (specified in the Link This Item To box). This information is identical to the quantitative analysis results that appear in the log window. The results will appear in the report only if the spectrum was the last to be quantified.
Peak Table	The peak finding results for the selected spectrum in the linked spectral window (specified in the Link This Item To box). This information is identical to the peak finding results that appear in the log window. The results will appear in the report only if the spectrum was the last to be used in a peak finding operation.
User Name	The name of the person who collected or processed the spectrum or information.
Chemical Structure	A chemical structure you have drawn and saved for the selected spectrum in the linked spectral window (specified in the Link This Item To box) using the Create/Edit Structures button on the Library Spectra tab of Library Manager.



Type	Description
OMNIC DDE Parameter	The name of an OMNIC DDE (dynamic data exchange) parameter. (These parameters are available in the OMNIC Macros\Pro software and let you specify items such as the number scans for data collection.) You will need to type the name of the parameter in the item in the Report Template window. See your OMNIC Macros\Pro documentation for information on OMNIC DDE parameters.
Search Result Picture	The green check mark or red X displayed by the search expert after a library search indicating the quality of the result.
QC Comparison Picture	The green check mark or red X displayed after a QC comparison indicating the quality of the result.
Signed By	The digital signature information for the last time the spectral data file was signed. This item can appear in a report only if you have the DS option.
Signature History	A record of the digital signature information for each time the report template was signed. This item can appear in a report only if you have the DS option.
Notebook File Name And Title	The file name and title of the current notebook.
System Status Results	The results of System Performance Verification tests, as shown in the Collection And Processing Information window.
QCheck Results	The results of a QCheck comparison.
Contour/Waterfall	The contour map or waterfall displayed in a map window using the OMNIC Atlas software.
Map Video Image	The video image of a sample that was saved when the displayed map was collected using the OMNIC Atlas software.
Map 3-D Image	The 3-D image of an area contour map displayed using the OMNIC Atlas software.

Follow these steps to add an item to a report template:

- 1. Use the arrow buttons in the Report Template window to display the page of the template that you want the item added to.**
- 2. Click the Add button in the Report Item box.**

The Add Report Item dialog box appears.

- 3. Specify the item type by selecting an option from the Type Of Report Item To Add drop-down list box.**

- 4. If desired, specify a font.**

You can specify a font for all of the types except Spectral Window, Clipboard Picture and Current Clipboard Picture. To do this, choose Font to display the Font dialog box, specify a font and then choose OK. The currently specified font appears to the left of the Font button.

- 5. If you selected the Spectral Window, Spectrum Title, Collection Time, Collection Information, Bench Configuration, Spectrum Comments or Spectrum History type, select a spectral window to which to link the item from the Link This Item To drop-down list box.**

To link the item to the spectral window that was active just before the Report Template window became active, select Active Spectral Window. When you print a report on paper, OMNIC places the current image from the specified window in the appropriate location. (The image shown in the report template is not updated when you change the contents of the linked window, but the printed report includes the changes.)

If you selected the Spectral Window type, the X-Axis Display Limits text boxes become available. See the next step.

If you selected any type other than Spectral Window, the Autosize options become available. These options let you automatically resize report template items or the boxes that contain the items. See step 7.

6. **If the X-Axis Display Limits text boxes are available, type in the text boxes the starting and ending X-axis limits of the spectral region you want to appear in the image of the spectral window.**

If you leave the text boxes blank, the spectrum will be displayed using the current display limits of the spectral window.

7. **If the Autosize options are available, select an option in the Autosize box.**

The following table describes each option.

Option	Description
None	Select this option if you don't want the item resized to fit the box or the box resized to fit the item when you manually change the size of either.
Size Content To Box	If you manually change the size of the box, the item is resized to fit the box. If the content is text, the font size is changed.
Size Box To Content	If you manually change the item text or its font size, the box is resized to fit the item.

**Note** If you select the Text, Prompt For Text, Clipboard Picture or Current Clipboard Picture type, only the None and Size Content To Box options are available. ▲

8. **Choose OK.**

The item appears in the upper-left corner of the page. Resize or move the added item as desired. See “Resizing and moving items.”

**Note** If you added a Prompt For Text item, you will be prompted to enter the text when you preview or print a report using the template. ▲

### About adding a chemical structure to a report

Be sure to follow the steps below to ensure that a chemical structure you have added to a report appears in the report:

1. **Select a report template that includes a Chemical Structure item.**

2. **Perform a search using a library that includes drawn chemical structures.**
3. **Select a library spectrum in the list of matches to display its structure.**

Close the Search window if desired.

4. **Select the searched sample spectrum in the linked spectral window.**

This is the window you specified as linked when you created the template.

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

The structure appears in the report.

**Note** Do not use Library Manager to display a different structure before previewing the report in step 5. ▲

## **Resizing and moving items**

When you are creating or editing a template, each item in the template is in a box. When you click an item to select it, an outline of the box appears with small, solid black “handles” at its corners and sides. Use these handles to resize or move an item.

Follow these steps to resize or move a report template item:

1. **Select the template item by clicking it in the Report Template window.**

If the item is covered by other items, first use the To Back button to move the other items behind the item of interest.

2. **If the item is a spectral window, or text for which Autosize in the Add Report Item dialog box or Change Report Item(s) dialog box has been set to Size Content To Box, you can change the item's size by resizing the box.**

To resize the width, drag a handle at the middle of the left or right side of the box. To resize the height, drag a handle at the middle of the top or bottom. To resize the width and height at the same time, drag one of the corner handles.

3. **If the selected item is text for which Autosize has been set to None or Size Box To Content, you can change the font size of the text by choosing Edit and using the Font button in the Change Report Item(s) dialog box.**

4. **To move an item, drag it to the desired location.**

You can also move a selected item or group of items by pressing the arrow keys on the keyboard. To move an item containing editable text, you must first deselect it (by clicking outside it) before dragging it to a new location.

## Deleting an item from a report template



When you are creating or editing a template, you can use the Delete button in the Report Item box to delete the selected item from the template. Follow these steps:

1. **Select the template item by clicking it in the Report Template window.**

If the item is covered by other items, first use the To Back button to move the other items behind the item of interest.

2. **Click the Delete button in the Report Item box.**

## Changing an item in a template



When you are creating or editing a report template, use the Edit button in the Report Item box to change a template item. Follow these steps:

### 1. Select the template item by clicking it in the Report Template window.

If the item is covered by other items, first use the To Back button to move the other items behind the item of interest.

**Note** If you want to change the item to a different type, you must first delete it and then add a new item of the desired type. ▲

You can select multiple items by holding down the Shift key and clicking the items. You should normally do this only for similar items.

**Note** You can double-click the item instead of selecting it and then choosing Edit in the next step. ▲

If the item type is Text, you can edit the text directly. Just click the text and use standard editing techniques. You can change the font in the next step.

### 2. Choose Edit.

The Change Report Item(s) dialog box shows the parameters appropriate for the type of item you selected. These parameters are the same as those you set in the Add Report Item dialog box.

### 3. If desired, specify a font.

You can specify a font for all of the types except Spectral Window, Clipboard Picture and Current Clipboard Picture: Choose Font to display the Font dialog box, specify a font and then choose OK. The currently specified font appears to the left of the Font button.

4. **If the item type is Spectral Window, Spectrum Title, Collection Time, Collection Information, Bench Configuration, Spectrum Comments or Spectrum History, select a spectral window to which to link the item from the Link This Item To drop-down list box.**

To link the item to the spectral window that was active just before the Report Template window became active, select Active Spectral Window.

When you print a report on paper, OMNIC places the current image from the specified window in the appropriate location. (The image shown in the report template is not updated when you change the contents of the linked window, but the printed report includes the changes.)

If the item type is Spectral Window, the X-Axis Display Limits text boxes are available. See the next step. If the item is any type other than Spectral Window, the Autosize options are available. These options let you automatically resize report template items or the boxes that contain the items. See step 6.

5. **If the X-Axis Display Limits text boxes are available, type in the text boxes the starting and ending X-axis limits of the spectral region you want to appear in the image of the spectral window.**
6. **If the Autosize options are available, select an option in the Autosize box.**

The following table describes each option.

Option	Description
None	Select this option if you don't want the item resized to fit the box or the box resized to fit the item when you manually change the size of either.
Size Content To Box	If you manually change the size of the box, the item is resized to fit the box. If the content is text, the font size is changed.
Size Box To Content	If you manually change the item text or its font size, the box is resized to fit the item.

**Note** If the item type is Text or Prompt For Text, only the None and Size Content To Box options are available. ▲

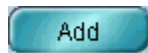
## Moving an item to the back



If a report item in the Report Template window obscures another item that you want to edit or move when you are creating or editing a report template, you can use the To Back button to move the first item to the back so that it is behind all the other items. Follow these steps:

1. **Select the template item by clicking it in the Report Template window.**
2. **Choose To Back.**

## Adding or deleting a page



When you are creating or editing a report template, use the Add and Delete buttons in the Page box in the Report Template window to add or delete a page from the template. The current page and total number of pages are indicated in the lower-right corner of the window.

To add a page, choose Add. The page is added at the end of the template.



To delete a page, first use the arrow buttons to display the page and then choose Delete. You can delete any page except page one.

## Saving a report template



Use the Save As button in the Report Template window to save on a disk the report template you are creating or editing. Follow these steps:

1. **Choose Save As in the Report Template window.**

A dialog box appears.

2. **Specify a filename and directory location for saving the template.**
3. **Type a description for the template in the Description box.**

Entering descriptions for templates makes it easier to select an appropriate template later.



## Selecting, editing or creating a report template

### 4. Choose Save.

Use Template in the Report menu to select a report template for printing reports or adding reports to a notebook, to edit a template, or to create a new template. See “Working with reports” for a discussion of using report templates, reports and report notebooks.

OMNIC includes several example report templates. These are in the C:\My Documents\OMNIC\Report directory (or other location where you installed OMNIC). To save time, we recommend that you modify one of these templates whenever you want to design a new template. Save the template with a new name after you make your changes.

**Notice** Use Options in the Edit menu to specify the margins and orientation for the template before you create a new template. You will not be able to change these items after you create the template. See “Print options” in the “Edit” chapter for details. ▲

If you use Template just to select a stored report template, that template becomes the current template. When you later print a report or add a report to a notebook, OMNIC automatically fills in 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.

If you use Template to edit a stored report template or to create a new template, the Report Template window provides the features you need.

The page number of the currently displayed page and the total number of pages in the template are shown in the lower-right corner of the Report Template window. To display a different page of the template, click the appropriate arrow button.

### — *How to* ➡

Select, edit or create a report template

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

A dialog box lists the available report template files. These files have the extension .RPT.

**Note** You can specify a default directory for this operation in the File options (available through Options in the Edit menu). (If you have the DS option, the directory is specified by the Directory For Report Templates And Notebooks system policy.) ▲

- 2. If you want to select a template to use for printing reports or adding reports to a notebook, or if you want to edit a stored template, type the name of the template file or locate and select a file.**

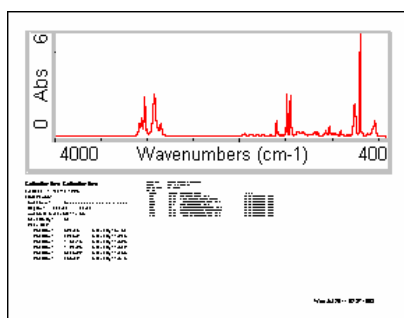
If you want to create a new template, go to step 5.

When you click the filename of a template, its description (if one exists) appears in the Description box. The description can help you select an appropriate template.

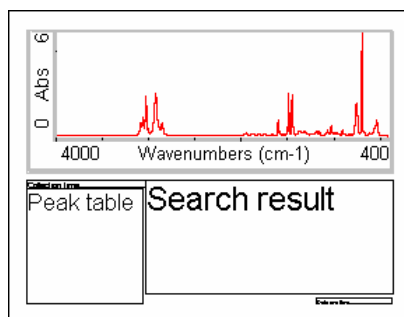
**Note for DS systems** If Prevent Changing Directories When Opening Files is selected in the system policies, you cannot change directories or drives to locate a file to select. ▲

A “preview” image of the selected template appears at the right side of the dialog box.

- To view the image in the form of a report filled in with information, select the Layout option below the image. This lets you see how the report will look when printed, although the text may be too small to read here.



- To view the image with identifying labels placed on report items that contain text (for example, “Search result” for a list of spectra found by a library search), select the Description option. This can make it easier to identify the types of items contained in the template.



**3. To select the template for later use, choose Select.**

The procedure is finished. The next time you print a report or add a report to a notebook, the template you just selected will be used.

**4. To edit the template, choose Edit.**

The Report Template window appears. You can begin changing the template with the features provided in the window. (See “Working with reports” for detailed instructions.) Go to step 6.

**5. To create a new template, choose Create.**

The Report Template window appears and you can begin adding items to the template with the features provided in the window.

**Note** We recommend that you modify one of the provided templates whenever you want to design a new template instead of creating a new template with the Create button. Save the template with a new name after you make your changes (see the next step). ▲

**6. When you are finished editing or creating the template, use the Save As button to save it.**

A dialog box lets you specify a filename and location for the template. Type a description of the template in the Description box. Entering descriptions for new templates makes it easier to select an appropriate template later (as explained in step 2 above). When you are finished, choose Save.

## 7. Close the Report Template window by clicking the Close button.

If you haven't saved your changes, a message asks whether to save them. Choose Yes to save the changes, No to close without saving, or Cancel to remain in the window.

To print a report using the template, choose Preview/Print Report from the Report menu.

## Previewing or printing a report

Use Preview/Print Report in the Report menu to view a report as it would appear on paper and print it. 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.

### — How to ➔

Preview or print a report

#### 1. Choose Preview/Print Report from the Report menu.

If the current template contains a Prompt For Text item, a message asks you to enter the text. Type the text in the text box and then choose OK.

An image of the report is displayed using the template. The page number of the currently displayed page and the total number of pages in the report are shown in the upper-right corner of the screen. To display a different page, click the appropriate arrow button.

To view an enlarged image of the report, choose Zoom. A scroll bar at the right lets you scroll portions of the report into view. To return to the normal view, choose Zoom again.

#### 2. If you want to use a different report template, choose Change Template.

A dialog box lets you select a report template file. Type the name of the file you want to use, or locate a file and select it by clicking its filename. A "preview" image of the selected template appears at the right side of the dialog box.

### Note for DS systems

If Prevent Changing Directories When Opening Files is selected in the system policies, you cannot change directories to locate a file to select. ▲

- To view the image in the form of a report filled in with information, select the Layout option below the image. This lets you see how the report will look when printed, although the text may be too small to read here.
- To view the image with identifying labels placed on report items that contain text, select the Description option. This can make it easier to identify the types of items contained in the template.

Choose Select. The selected template appears in the report preview screen with the items filled in where appropriate.

### 3. To print the report, choose Print.

The Print dialog box lets you specify items such as the number of pages to print. Set the parameters as desired and then choose OK. (See your Windows documentation for more information.) The report is then printed.

**Note** Use the Print options (available through Options in the Edit menu) to specify how to print the spectra in a report. For example, you can specify fonts and line thickness. ▲

### 4. Choose Close to remove the report preview from the screen.

## Creating a new report notebook

Use New Notebook in the Report menu to create a new report notebook to which you can add reports.

### ■ *How to* ➡

Create a new report notebook

1. **Choose New Notebook from the Report menu.**
2. **In the dialog box that appears, enter a filename for the new notebook and specify a directory location for the file.**
3. **Choose OK.**

## Adding a report to a notebook

Use Add To Notebook in the Report menu to add a report to a report notebook. The information contained in the report depends on the template you use for the report. After you add a report to a notebook, you can use View Notebook in the Report menu to see the report within the notebook, print a report or retrieve a spectrum from a report. See “Viewing and using report notebooks” for details.

### — How to ➡

Add a report to a notebook

#### 1. Choose Add To Notebook from the Report menu.

An image of the current report is displayed as it will appear on paper.

The pathname of the current notebook appears near the top of the screen. To view a different page, click the appropriate arrow button. To enlarge the report, choose Zoom. A scroll bar at the right lets you scroll portions of the report into view. To return to the normal view, choose Zoom again.

#### Notice

Once you add a report to a notebook, you cannot delete the report or change its template. The next two steps explain how to change the template or notebook before adding the report to a notebook. ▲

#### 2. To use a different report template, choose Change Template.

A dialog box lets you select a report template file. Type the name of the file you want to use, or locate a file and select it by clicking its filename. Choose Select. The selected template then appears with the items filled in where appropriate.

#### Note for DS systems

If Prevent Changing Directories When Opening Files is selected in the system policies, you cannot change directories to locate a report template. ▲

#### 3. If you want to add the report to a different report notebook or create a new notebook, choose Change Notebook.

A dialog box lets you select a report notebook file or create a new notebook. To use an existing notebook, type its filename, or locate a file and select it by clicking its filename. To create a new notebook, enter a new filename. Choose Open. The specified notebook becomes the current notebook.

**Note for DS systems** If Prevent Changing Directories When Opening Files is selected in the system policies, you cannot change directories or drives to locate a notebook. ▲

**Note** You can also create a new notebook by using New Notebook in the Report menu. ▲

#### 4. Choose Add To Notebook.

A dialog box asks for a descriptive title for the report.

#### 5. Type a title in the text box.

#### 6. If you are sure you want to add the report to the current notebook using the current template, choose OK.

*You will not be able to delete the report from the notebook or change its template after you choose OK.*

The next time you view the notebook, the report you added will be available.

**Note for DS systems** You may be prompted to digitally sign a file during this step. Follow the instructions that appear on the screen. ▲

## Viewing and using report notebooks

OMNIC lets you save your work in the form of reports that you can add to one or more report notebooks. A report notebook is similar to a laboratory notebook: it is a permanent record of the results of your spectroscopy work arranged in chronological order. For example, you can use a notebook to archive reports that contain sample spectra and their library search results or quantitative analysis results.

After you have added one or more reports to a notebook, you can page through them to find a report created on a particular date or use the text search feature to find reports related to a topic of interest. You can print reports from a notebook at any time, but you cannot edit or delete them.


You will find that saving reports in report notebooks saves you time—and paper—by eliminating the need to recreate reports or to store printed copies of them in a file cabinet.

To view a report notebook, use View Notebook in the Report menu. After you select the notebook you want to view, OMNIC displays it in the form of a notebook with three labeled tabs along the right side. When you click a tab, the related information and features are brought to the front of the notebook.

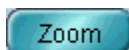
The **Table Of Contents** tab lists the reports in the notebook and shows when the reports were added. See “Using the table of contents” for details.

The **Search For Text** tab lets you find reports by searching for text they contain or for the date they were added to the notebook. See “Searching for text” for details.

The **Reports** tab lets you view reports contained in the notebook. See “Paging through reports” for details.

A blue button with rounded corners and a slight shadow, containing the text "Change Notebook" in white.

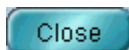
Near the top of the notebook are buttons that let you perform various operations. You can use the Change Notebook button to view a different notebook at any time. While you are viewing a report, you can use the Print button to print individual report pages and use the Zoom button to enlarge or shrink the display of information.

A blue button with rounded corners and a slight shadow, containing the text "Print" in white.A blue button with rounded corners and a slight shadow, containing the text "Zoom" in white.A blue button with rounded corners and a slight shadow, containing the text "Copy" in white.

You can use the Copy button to copy the selected or displayed report to the Windows Clipboard. If the Table Of Contents tab is displayed, select the desired report in the list and then choose Copy. If the Reports tab is displayed, choose Copy to copy the displayed report. You can then paste the copied report into a document using an application that accepts items from the Clipboard.

A blue button with rounded corners and a slight shadow, containing the text "Sign" in white.

If you have the DS option, the Sign button appears on the Table Of Contents tab and Reports tab. You can use the button to add a digital signature to reports in the notebook. See “Signing a report” for details.

A blue button with rounded corners and a slight shadow, containing the text "Close" in white.

When you are finished viewing the notebook, click the Close button.



## Signing a report



If you have the DS option, you can use the Sign button to digitally sign a report in the displayed notebook. The visible portion of a digital signature consists of a user name, a date and a stated reason for signing. A digital signature also contains encrypted information that guarantees that the file has not changed since it was signed and that the file can be changed only by a user who enters the correct name and password.

If you are viewing the Table Of Contents tab of the notebook, select the report you want to sign in the list and then choose Sign. If you are viewing the Reports tab, use the Report scroll bar or the Page buttons to display the report you want to sign and then choose Sign. Follow the instructions that appear on the screen.

## Using the table of contents

The reports contained in the current notebook are listed on the Table Of Contents tab.

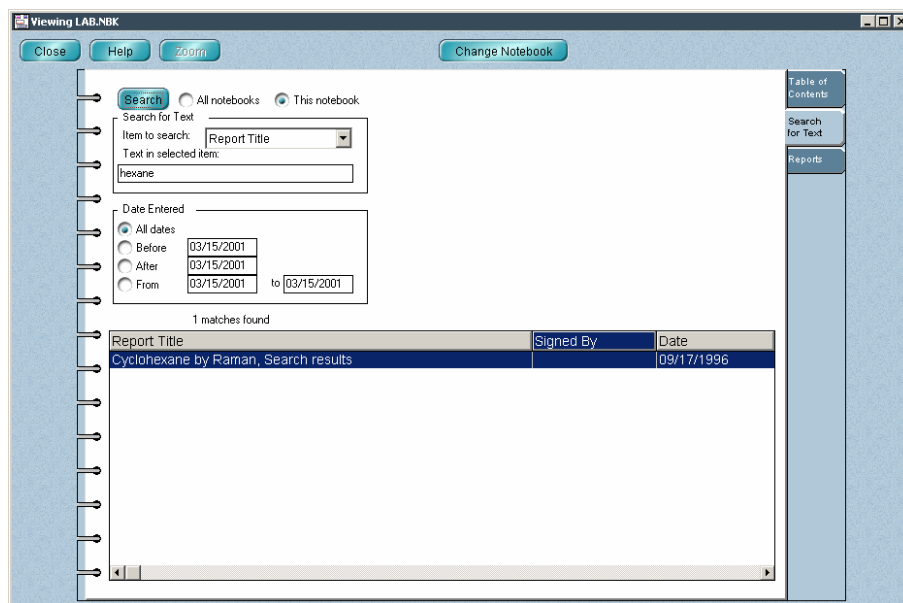
Report Title	Signed By	Date
2-Bromopropane analysis		Sep 16, 1996
Cyclohexane by Raman, Search results		Sep 17, 1996
Methanol by ATR analysis		Sep 18, 1996
Oil analysis that contains gasoline		Sep 19, 1996
Aspirin QC verification		Sep 20, 1996
Polystyrene by thin film		Sep 23, 1996
Unknown drug sample analysis		Sep 24, 1996
Report with chemical structure		Dec 03, 1996

You can list them in alphabetical order by their titles or chronologically by their dates of creation by clicking the appropriate column heading. If you have the DS option, you can list the reports by their digital signatures by clicking the Signed By column heading. To see more of the information in the cells of a column, you can drag the vertical dividing lines between the column headings to the left or right to change the width of the column.

To view a report, double-click it in the list. The report is then displayed on the Reports tab.

## Searching for text

Click the Search For Text tab of the report notebook if you want to find reports by searching for text they contain.



You can find text in any report item available in the Item To Search dropdown list box provided that the item is in a report. (See the table below for a description of the items.) These are the items you added to your report templates when you created or edited them.

Item	Description
All Items	All report items that contain searchable text.
Report Title	The title of the report.
Text	Text that you can edit directly in the Report Template window.
Date And Time	The date and time when the report was created.
Search Result	The results of a spectral search or QC comparison.
Peak Table	The results of a peak finding operation.
Quant Result	The results of a quantitative analysis performed with the Quantify command.
Prompt For Text	Text entered when the report was previewed before being added to the notebook.

Item	Description
Spectrum Title	The title of a spectrum in a linked spectral window.
Collection Time*	The date and time a spectrum in a linked spectral window was collected.
Collection Information*	The data collection information for a spectrum in a linked spectral window. This includes the number of sample and background scans and the resolution, gain, velocity and aperture values.
Bench Configuration*	The spectrometer configuration information for a selected spectrum in a linked spectral window. This includes the detector, beamsplitter and source.
OMNIC DDE Parameter	The name of an OMNIC DDE (dynamic data exchange) parameter. See your OMNIC Macros\Pro documentation for information on OMNIC DDE parameters.
Spectrum Comments*	The comments for a spectrum in a linked spectral window. These are the same comments as are displayed in the Collection And Processing Information window for the spectrum.
Spectrum History*	The data processing history of a spectrum in a linked spectral window.
User Name	The name of the person who collected or processed a spectrum or information.
Signed By	The digital signature information for the last time the spectral data file was signed. This item can appear in a report only if you have the DS option.
Signature History	A record of the digital signature information for each time the spectral data file was signed. This item can appear in a report only if you have the DS option.

\* The item must be in the report. If only the linked spectral window is in the report, the text will not be found.

Follow these steps to search for text in reports:

**1. Click the Search For Text tab of the notebook.**

The name of the current notebook is shown in the title bar.

**2. If you want to search only this notebook, select This Notebook. If you want to search all the notebooks, select All Notebooks.**

If you want to search a different notebook by itself, use the Change Notebook button to locate and select it.

**Note for DS systems**

If Prevent Changing Directories When Opening Files is selected in the system policies, you cannot change directories or drives to locate a notebook to select. ▲

**3. Specify whether to search for text in one template item or in all items by selecting an option from the Item To Search drop-down list box.**

**4. Type the text to search for in the Text In Selected Item box.**

**5. To search all reports, select All Dates in the Date Entered box. To search only reports added before a certain date, select Before and enter the date in the corresponding text box.**

The options in the Date Entered box let you limit the search to reports added to a notebook during a specified time period.

Express dates on this tab in the format used by your system. For example, in the U.S.A. this is normally month/day/year, with the month and day as two-digit numbers and the year as a four-digit number. To search only reports added after a certain date, select After and enter the date in the text box. To search only reports added during a certain period, select From \_\_\_ To \_\_\_ and enter the starting and ending dates.

## 6. Choose Search.

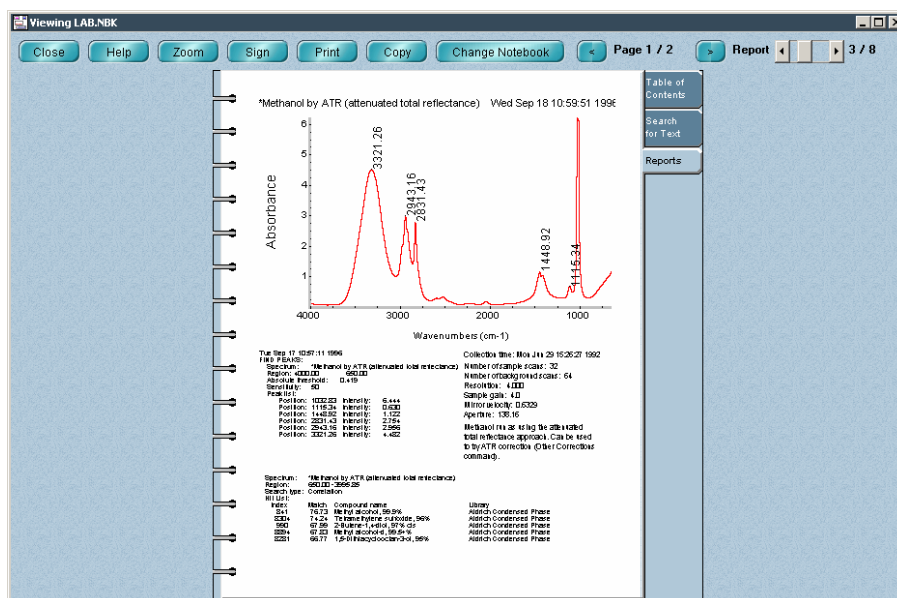
The number of reports found is displayed below the Date Entered box, and the search results appear in the table. To list the found reports in alphabetical order by title, click the Report Title column heading. To list the reports in chronological order, click the Date column heading. If you have the DS option, you can list the reports by their digital signatures by clicking the Signed By column heading. To see more of the information in the cells of a column, you can drag the vertical dividing lines between the column headings to the left or right to change the width of the column.

To view a found report, double-click its row in the table. The Reports tab displays the information.

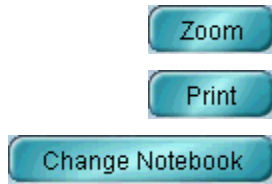
## 7. Choose Close to close the notebook if desired.

## Paging through reports

Click the Reports tab of the notebook to view individual reports as they would appear on paper. (You can also double-click a report title on the Table Of Contents tab to display a report.)



The Report scroll bar and Page buttons let you browse through the reports and report pages.



To enlarge your view of the information, use the Zoom button. To print a report, use the Print button. To view a different notebook, use the Change Notebook button.

### — *How to* ➔

View or use a report notebook

#### 1. **Choose View Notebook from the Report menu.**

The Select Report Notebook dialog box lets you select a report notebook file.

#### 2. **Type the name of the file you want to view, or locate a file and select it by clicking its filename.**

#### **Note for DS systems**

If Prevent Changing Directories When Opening Files is selected in the system policies, you cannot change directories or drives to locate a file to select. ▲

#### 3. **Choose OK.**

The report notebook appears with the table of contents displayed. To list the reports in the notebook in alphabetical order by their titles, click the Report Title column heading. To list them chronologically by their dates of creation, click the Date column heading. If you have the DS option, you can list the reports by their digital signatures by clicking the Signed By column heading. To see more of the information in the cells of a column, you can drag the vertical dividing lines between the column headings to the left or right to change the width of the column. See “Using the table of contents” for more information.

#### 4. **To view a report, double-click its title.**

The Reports tab is brought to the front displaying the report. You can also click the Reports tab to view it. See “Paging through reports” for more information.

You can use the Report scroll bar or click the Page arrow buttons near the top of the window to page through reports in the notebook.

To expand the display of a report for easier viewing, choose Zoom. Choose Zoom again to return the report to its normal size.

If a report contains an image of a spectral window, you can double-click the image to display the spectra in a spectral window.

To print the displayed report, choose Print.

To copy the displayed report to the Windows Clipboard, choose Copy. You can also copy a report by selecting it in the list on the Table Of Contents tab and choosing Copy. Once a report is copied, you can paste it into documents using other applications that use the Clipboard.

If you want to view reports in another notebook, choose Change Notebook. In the dialog box that appears locate and select the desired notebook and then choose OK.

**Note for DS systems**

If Prevent Changing Directories When Opening Files is selected in the system policies, you cannot change directories or drives to locate a notebook to select. ▲

**5. To search for reports that contain particular text, click the Search For Text tab and use its features.**

See “Searching for text” for complete information.

**6. To add a digital signature to a report, use the Sign button on the Table Of Contents tab or Reports tab.**

The Sign button is available only if you have the DS option.

**7. When you are finished viewing the notebook, choose Close.**





# Window

The Window menu includes commands for working with windows on the screen. The primary use of each command is summarized in the following table:

To do this...	Use this command...
Create a new spectral window.	New Window
Display spectral windows in a tiled arrangement.	Tile Windows
Display spectral windows in a layered arrangement.	Cascade Windows

The title of every window is listed at the bottom of the Window menu. You can select any of these windows by choosing its title from the Window menu.

## Creating a new spectral window

Use New Window in the Window menu to create a new spectral window. The window becomes the selected window.

The way panes, axes and other features are displayed in the new window is determined by the settings of the Window options (available through Options in the Edit menu). See “New Window options” in the “Edit” chapter for information on setting these options.

### ■ *How to* ➔

Create a new spectral window

#### **Choose New Window from the Window menu.**

If Prompt for New Window Title is turned on in the Window options (available through Options in the Edit menu), a dialog box asks for a title for the new spectral window. Type a title and then choose OK. See “New Window options” in the “Edit” chapter for more information on the Prompt for new window title option.

A new spectral window appears on the screen. Its appearance depends on the settings of the Window options (available through Options in the Edit menu).

## Tiling windows

Use Tile Windows in the Window menu to resize and rearrange all of OMNIC's displayed windows so that they fill the OMNIC window without overlapping, like floor tiles (see the following example). (Minimized windows, the Collection And Processing Information window and windows opened using other applications are not tiled.) The windows are automatically resized and reshaped as needed to make them fit. Rearranging the windows in this way lets you see all of the spectral windows at the same time and lets you easily move between windows when there are many on the screen.



**Note** When windows are tiled, they may be too small to allow you to see the displayed information clearly. ▲

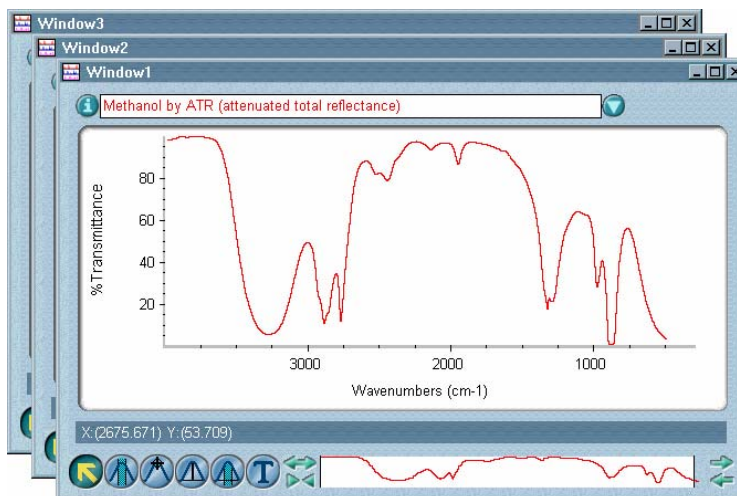
### — How to ➡

Tile windows

**Choose Tile Windows from the Window menu.**

## Cascading windows

Use Cascade Windows in the Window menu to resize and layer all of OMNIC's displayed windows and arrange them within the OMNIC window so that their title bars are visible. Here is an example:



### — How to —>

Cascade windows

**Choose Cascade Windows from the Window menu.**



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