IR SERIES

Nicolet IR100 and Nicolet IR200 User's Guide

For Technical Support, please contact:
Thermo Fisher Scientific
5225 Verona Road
Madison WI 53711-4495 U.S.A.
Telephone: 1 800 532 4752
E-mail: us.techsupport.analyze@thermofisher.com
World Wide Web: http://www.thermo.com/spectroscopy

For International Support, please contact:
Thermo Fisher Scientific
Telephone: +1 608 273 5017
E-mail: support.madison@thermofisher.com
World Wide Web: http://www.thermo.com/spectroscopy

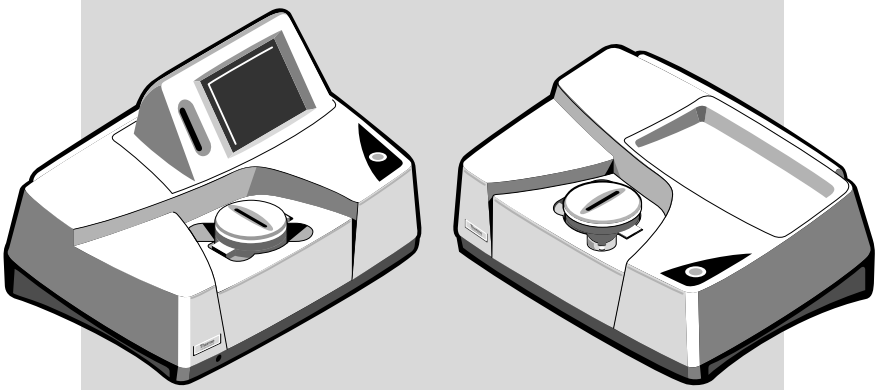
269-107302, Rev B

Contents

Welcome

Congratulations on your purchase of a Thermo Scientific Nicolet™ IR100 or Nicolet IR200 spectrometer! These compact instruments let you collect and process infrared spectra of a wide variety of samples with easy-to-use Encompass™ software.

Note If you have a Spectronic IR100, follow the instructions given for the Nicolet IR100. ▲



The Nicolet IR100 includes a built-in computer and display that lets you view the spectra you collect and process. The Nicolet IR200 uses a desktop computer and display monitor for collecting and processing spectra with Encompass, or with the versatile EZ OMNIC™ software package.

Nicolet IR100 flexibility

You can also use your Nicolet IR100 with a desktop computer. Simply purchase Encompass or EZ OMNIC for the PC, install it on the computer, and connect the computer to the spectrometer as explained for the Nicolet IR200 in the manual titled *Installing Your Spectrometer*. Then follow the instructions given in this manual for the Nicolet IR200. ▲

Before you install or use your system, read the *Spectrometer Safety Guide* (see the following Warning). To install the spectrometer, follow the instructions in the manual titled *Installing Your Spectrometer*. Then read the "Getting Started" chapter of this manual to learn the basics of the system. See "Where to find the information you need" later in this chapter for a description of the printed and on-line documentation provided with the system.

Note

If you purchased a Transport Kit, use the manual titled *Transport Kit User's Guide* in conjunction with the instructions in this manual that apply to the Nicolet IR100. All of the features of the Transport Kit and the Nicolet IR100 are the same except for the special features described in *Transport Kit User's Guide*. That manual describes the environmental conditions under which you can use the Transport Kit and explains how to set up the spectrometer. ▲

⚠ Warning

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

The Nicolet IR100 and Nicolet IR200 spectrometers are Class I laser products. The accessible radiation levels during normal use and maintenance for the Nicolet IR100 and Nicolet IR200 are below limits defined by the United States Department of Health and Human Services and international laser safety standards. The Nicolet IR100 and Nicolet IR200 comply with FDA performance standards for laser products except for deviations pursuant to Laser Notice 50, dated July 26, 2001.

⚠ Caution Use of controls or adjustments or performance of procedures other than those specified in the provided spectrometer documentation may result in hazardous radiation exposure. ▲

Important To avoid damage to the spectrometer cover, do not allow it to come into contact with aggressive solutions or harsh chemicals such as acetone, tetrohydrofuran or acetonitrile. ▲

Using this manual

This manual explains how to use your Nicolet IR100 or Nicolet IR200 spectrometer with Encompass. If you have a Nicolet IR200, EZ OMNIC is also available. See the documentation that came with that software for information on using its features.

If you have a Nicolet IR100 with the optional touch screen, you will use a stylus to touch items on the screen rather than click them using a mouse. You can store one of the provided styluses in the groove at the top of the touch screen housing. For convenience, in this manual we will use the term "click" alone except when an action using a stylus requires explanation. You can "double-click" an item on the touch screen by touching the item twice in rapid succession.

While the illustrations in this manual show the Nicolet IR100 spectrometer, all of the information, both written and pictorial, applies to both the Nicolet IR100 and Nicolet IR200 unless otherwise indicated.

This manual includes safety precautions and other important information presented in the following format:

Note Notes contain helpful supplementary information. ▲

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

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

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

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

System requirements

The Nicolet IR100 spectrometer includes everything that is needed for running Encompass.

To run Encompass on a Nicolet IR200 spectrometer, your system must meet these minimum requirements:

- Intel® Pentium® II processor with 233 MHz clock speed.
- 64 megabytes of random access memory (RAM).
- USB interface for spectrometer communication.
- Hard disk size of 2.0 gigabytes.
- Quad speed CD-ROM drive.
- 4 megabytes of video RAM.
- 1.44-megabyte floppy disk drive for 3.5-inch floppy disks.
- 15-inch SVGA monitor with 800-by-600 resolution.
- Keyboard and mouse.
- Appropriate printer port if you plan to print on a local printer.
- Windows® 98, Windows 2000, Windows Me or Windows XP. You must have Internet Explorer 5.0 or greater if you are using Windows 98.

If you have a Nicolet IR200 and did not purchase your computer from us, you will need to install Encompass. See the installation instructions that came with the software for more information.

To see the requirements for running EZ OMNIC, choose OMNIC Help Topics from the Help menu of EZ OMNIC, find "requirements" in the Index, and go to the "Recommended hardware and software for OMNIC" topic.

Where to find the information you need

The printed and on-line documentation included with your system is designed to help you find the information you need quickly. Your documentation set includes some or all of the following manuals and on-line Help (see the next section for more information about Help).

Preparing Your Site explains how to prepare your site for installing the Nicolet IR100 or Nicolet IR200 spectrometer. Information about the system dimensions, weight, electrical requirements, etc. is included.

Installing Your Spectrometer explains how to install the Nicolet IR100 or Nicolet IR200 spectrometer. The clearly illustrated steps make the installation easy.

Spectrometer Safety Guide covers safety considerations for the Nicolet IR100 and Nicolet IR200 spectrometers. Before using the system, be sure to read the entire guide. Always follow the precautions the guide contains whenever you use the system.

The *Nicolet IR100 and Nicolet IR200 User's Guide* (this manual) explains how to use the system to collect and work with FT-IR spectra. Included is information on spectrometer components, complete instructions for using the software features, and chapters on using accessories and troubleshooting problems.

The *Encompass Macros User's Guide* explains how to use Encompass Macros to create macros for performing many spectroscopy tasks with the software.

Servicing Your Spectrometer explains how to maintain and service the Nicolet IR100 and Nicolet IR200 spectrometers. Included are procedures for troubleshooting and replacing components, as well as a section in which you can record the maintenance and service procedures you have performed.

Replacement Parts for the Nicolet IR100 Spectrometer and *Replacement Parts for the Nicolet IR200 Spectrometer* provide part numbers for replacement parts you can order from us.

If you have a Nicolet IR200 with EZ OMNIC, you can view Getting Started With EZ OMNIC, a tutorial available through Getting Started in the Help menu. It provides a quick overview of the software features. In addition, the software's on-line Help system lets you quickly find answers to your questions about using all the features. To view the comprehensive *OMNIC User's Guide*, 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 OMNIC User's Guide. (Some features described in the guide are not available in EZ OMNIC.)

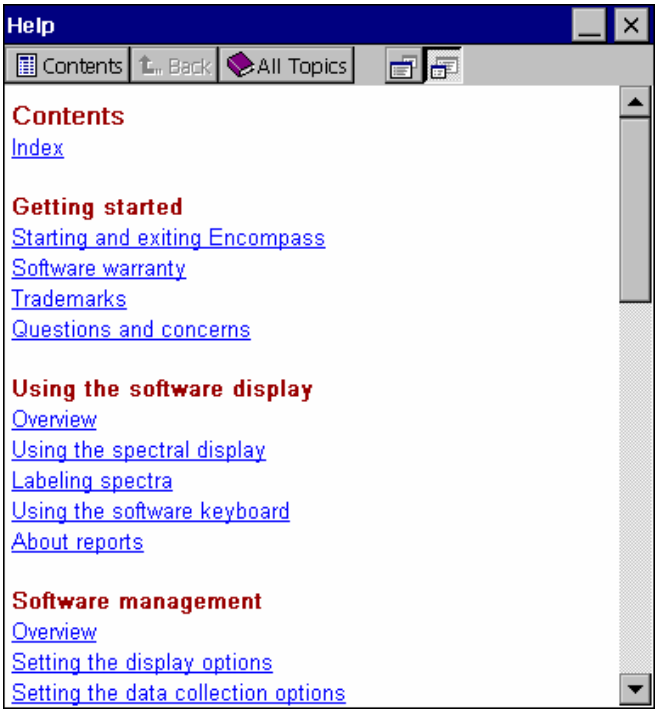
On-line Help

The on-line Help provided with Encompass lets you quickly find answers to your questions about using the software features. The next sections give details for using the Help system in each application.

Help for Nicolet IR100 systems

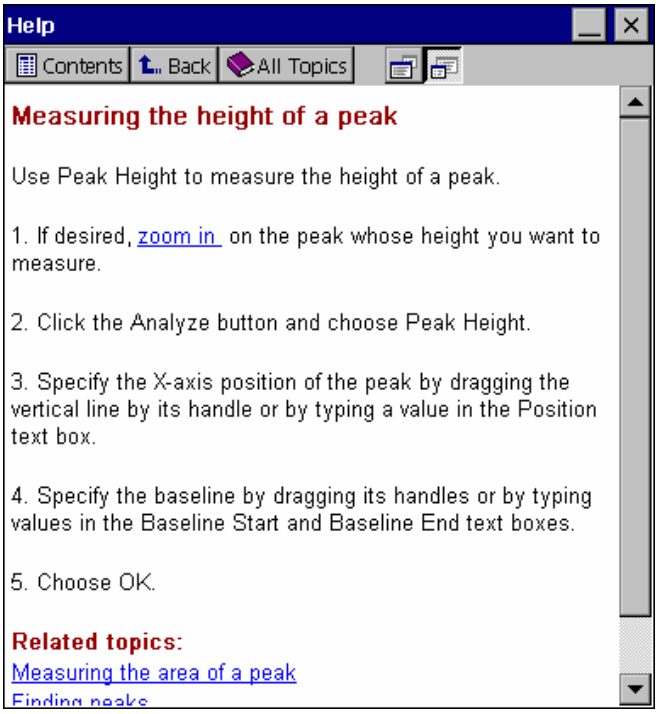
The Encompass Help system on a Nicolet IR100 spectrometer provides brief explanations of the software features. These instructions will be adequate for most situations. If you ever need more detailed information, please refer to this manual.

To display Help information from the main Encompass window, click the Help button. The table of contents appears showing the titles of available topics:



To view a topic, click its title.

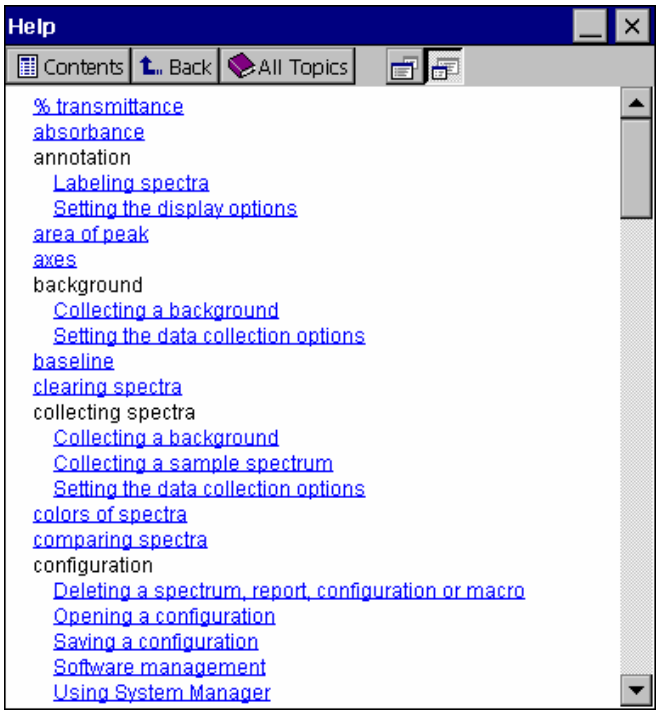
To display Help information for a dialog box or window you are using, click the provided Help button. A topic containing information about the features appears. Here is an example:



From the displayed topic you can go to other topics by clicking the underlined text.

To display the Help index, click the underlined word “Index,” which appears at the top of the table of contents and at the bottom of every topic. The index lists subjects in alphabetical order, with relevant topics shown below each subject.

You can use the scroll bar at the right to scroll subjects into view.

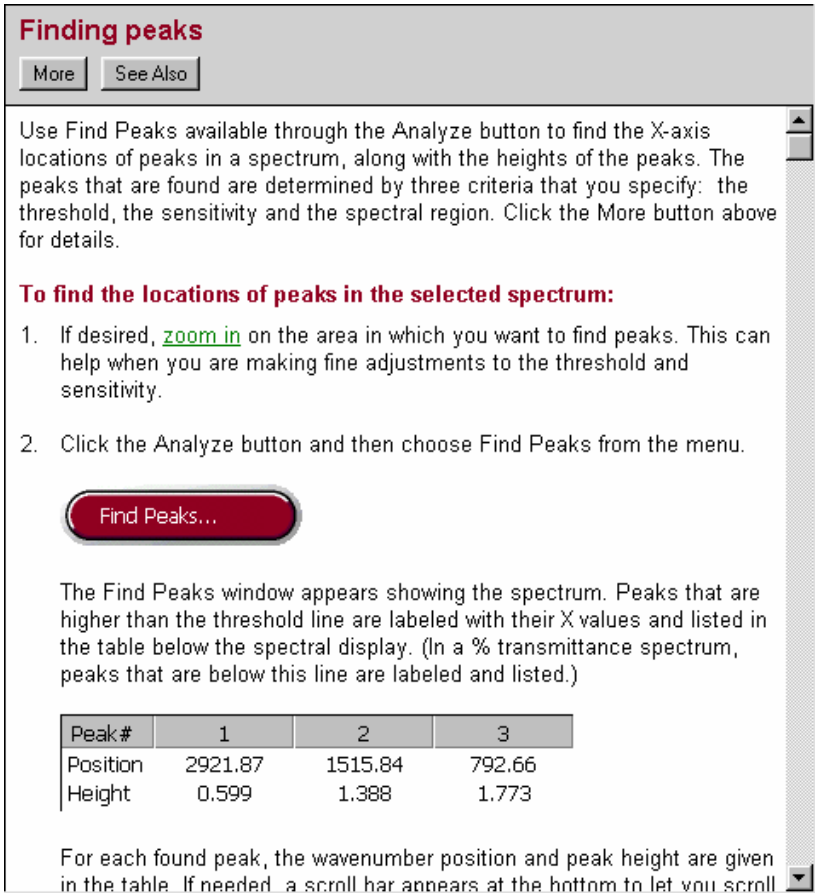


When you find the subject of interest, click the desired topic below it.

Help for Nicolet IR200 systems

The Encompass Help system for a Nicolet IR200 spectrometer provides detailed explanations of the software features. These instructions are very similar to the instructions in this manual.

To display Help information for a dialog box or window you are using, click the provided Help button. A topic containing information about the features appears. Here is an example:



Finding peaks

More | See Also

Use Find Peaks available through the Analyze button to find the X-axis locations of peaks in a spectrum, along with the heights of the peaks. The peaks that are found are determined by three criteria that you specify: the threshold, the sensitivity and the spectral region. Click the More button above for details.

To find the locations of peaks in the selected spectrum:

1. If desired, zoom in on the area in which you want to find peaks. This can help when you are making fine adjustments to the threshold and sensitivity.

2. Click the Analyze button and then choose Find Peaks from the menu.

The Find Peaks window appears showing the spectrum. Peaks that are higher than the threshold line are labeled with their X values and listed in the table below the spectral display. (In a % transmittance spectrum, peaks that are below this line are labeled and listed.)

Peak#	1	2	3
Position	2921.87	1515.84	792.66
Height	0.599	1.388	1.773

For each found peak, the wavenumber position and peak height are given in the table. If needed, a scroll bar appears at the bottom to let you scroll

From the displayed topic you can go to other topics by clicking underlined text within the topic or by using the buttons below the topic heading or below the Encompass Help window menu bar.

Click the Back button to return to previously displayed topic.

Click the Print button to print the current topic.

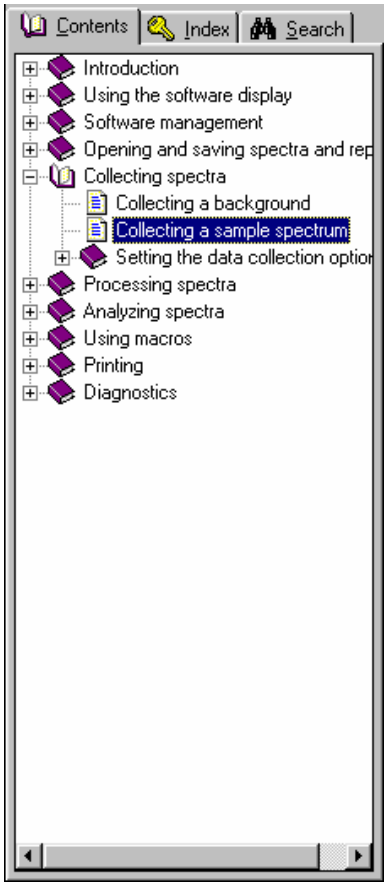
Click the left browse button to display the previous topic in the topic sequence you are browsing.

Click the right browse button to display the next topic in the sequence.

Click the Exit button to close the Help system.

Click the See Also button to display a list of related topics that you can then click to display.

Click the More button to display more general information about the command being discussed.



At the left side of the Encompass Help window is a pane containing three tabs. Click the tab you want to use.

The **Contents** tab displays books containing related topics about software features. To open a book, click the + sign next to it or double-click the book. To display a topic within a book, click the topic page icon. To close an open book, click the - sign next to it or double-click the book.

The **Index** tab lets you find topics by searching for subjects. You can type a subject in the text box at the top or scroll through the listed subjects. To display a topic, select the desired subject in the list. If more than one topic is associated with a subject, a list of topics pops up. Click the desired topic to display it.

The **Search** tab lets you find topics by searching for text. Click the Next button and then follow the instructions in the Find Setup Wizard to compile a list of all the words that appear in the Help system. You can type a word in the text box at the top or scroll through the listed words and select one. A list of topics that contains the word appears at the bottom. Select the desired topic to display it.

To display Help information from the main Encompass window, click the Help button and then use the tabs described above to locate the desired topic.

Accessories

A number of Spectra-Tech Foundation Series™ accessories, such as those listed below, are available for the Nicolet IR100 and Nicolet IR200 spectrometers.

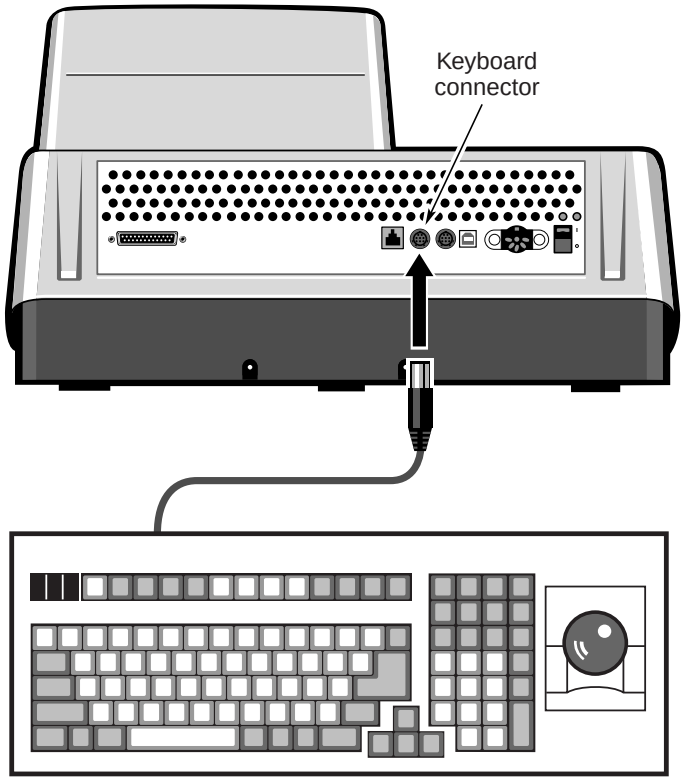
- SpeculATR™ accessory
- Multi-Bounce accessory
- Thunderdome™ accessory
- Endurance™ accessory
- Performer™ accessory

Each accessory comes with a manual explaining how to install and use it.

For more information about these accessories, contact Technical Support. See the “Questions and concerns” section later in this chapter for more information.

Using an external keyboard with a Nicolet IR100

If your Nicolet IR100 has a “Keyboard” connector on the rear panel, you can use it to connect a standard computer keyboard to the spectrometer.



This lets you enter any needed text into software prompts and dialog boxes using a full size keyboard instead of the software keyboard provided in Encompass. (See “Using the software keyboard” in the “Using the Software Display” chapter for information about the software keyboard.)

Note Some keyboard models may not be compatible with the Nicolet IR100. ▲

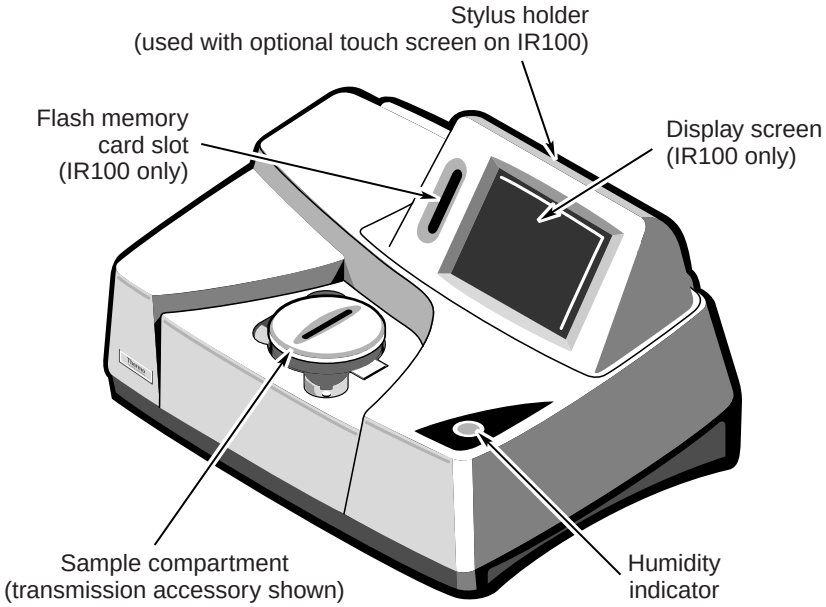
Questions and concerns

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.

Getting Started

This chapter identifies some major components of your spectrometer and explains how to turn on the system components and start and exit the software.

The illustration below shows some important components that are visible on the outside of the spectrometer.



⚠ Warning To avoid injury, always follow the safety precautions described in this manual and in the *Spectrometer Safety Guide* that came with your system. ▲

Turning on the system components

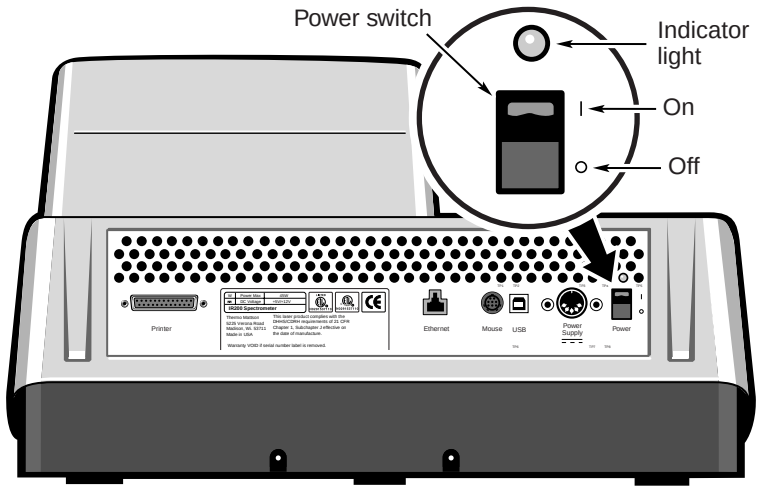
We recommend that you keep your spectrometer on at all times, unless the building is subject to power outages or you need to perform a service or maintenance procedure. Leaving the system on keeps it stable and gives you the most consistent results.

Important Do not turn on the spectrometer power until you have first connected the power cable to the spectrometer and then plugged it into a wall outlet or power strip. Sudden power surges can cause serious damage to the spectrometer. ▲

Follow these steps:

1. **Turn on the spectrometer power.**

   The power switch is on the rear panel of the spectrometer.



   An indicator light above the power switch indicates that the spectrometer (and laser) power is on. See the “Laser Safety” chapter of the *Spectrometer Safety Guide* for information on the laser power level.

   Let the spectrometer stabilize for at least 15 minutes (one hour for best results) before collecting spectra.

2. **If your system includes a printer, turn it on.**

3. **If you have a Nicolet IR200, turn on the computer and monitor.**

   Reverse the order given in this procedure when you turn off the system components.

Starting the software

The procedure for starting Encompass varies depending on whether you have a Nicolet IR100 or Nicolet IR200 and whether you are required to log in. See the next sections for instructions for starting the software and logging in.

Starting Encompass on a Nicolet IR100

If you have a Nicolet IR100, follow the steps below to start Encompass.

1. **Turn on the spectrometer power.**

   See "Turning on the system components" earlier in this chapter for details. Normally the power should be left on.

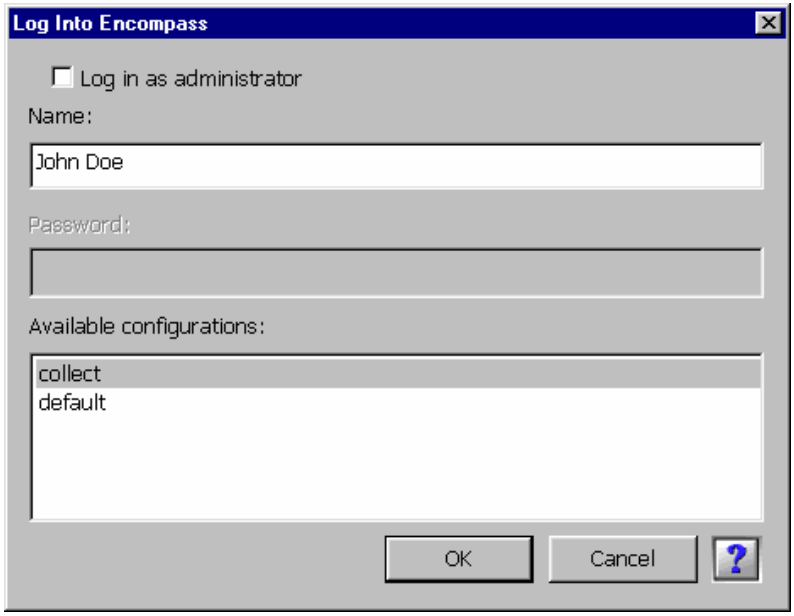
   Encompass starts when you turn on the power.

Note If the system clock needs to be set, a prompt appears allowing you to enter the current date and time using standard Windows features. The clock is used for purposes such as recording when data collection and processing operations are performed. If you need help setting the clock, contact your system administrator. ▲

   If you are not prompted to log in by entering your name, the procedure is finished and you can now use the software. Otherwise, go to the next step.

2. **If you are prompted to log into Encompass, enter your user name and select a configuration or macro if any are listed.**

   Type your user name in the Name text box. Click inside the text box to display the software keyboard.



The appearance of this dialog box varies depending on how the software has been set up and which model spectrometer you have.

   If you want to log in as the system administrator, turn on the Log In As Administrator check box. You must also enter the administrator's password in the Password text box (see the Note below). The administrator is given access to software options that control how the system is used. See "Using System Manager" in the "Software Management" chapter for details.

Note When you first use the software, no administrator password exists. In this situation, do not enter anything in the Password text box if you are logging in as the administrator. Then use System Manager available through the Setup button to enter the desired password. See "Using System Manager" in the "Software Management" chapter for more information. ▲

If the system has been set up to allow access only to certain configurations, they are listed in the Allowed Configurations box. Select the desired configuration by clicking it. See the "Software Management" chapter for information about configurations.

If the system has been set up to use macro mode, the available macros are listed in the Available Macros box (it appears instead of the Available Configurations box). Select the desired macro by clicking it. This macro will start when you choose OK to close the Log Into Encompass dialog box in the next step. See "Macro mode" in the "Software Management" chapter for more information about macro mode.

3. **Choose OK.**

   You can now use the software.

   If the system has been set to use macro mode, the macro you selected in step 3 starts running. Respond appropriately to any prompts that appear. (See the "Running a Macro" chapter of the Encompass Macros User's Guide for more information on running a macro.) When the macro is finished running, the Log Into Encompass dialog box reappears, allowing you to run another macro (see step 3). Another user or the administrator can also log in at this time.

Collecting your first spectrum

If you are using the system for the first time and want to collect your first spectrum, read the "Collecting Spectra" chapter now. ▲

Starting the software on a Nicolet IR200

If you have a Nicolet IR200 spectrometer, follow the steps below to start Encompass. If you are using EZ OMNIC, see the on-line documentation that came with the software for instructions.

Note If your system includes EZ OMNIC and a DTGS detector, you must use Configure Bench on the Diagnostic tab of the Experiment Setup dialog box (available in the Collect menu) to set the Detector parameter to DTGS KBr (instead of the standard lithium tantalate detector). ▲

1. **Start Windows.**

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

Note Your network administrator can connect the system computer to a network in the same manner as any other computer running Windows. ▲

2. **Double-click the Encompass shortcut on the Windows desktop.**

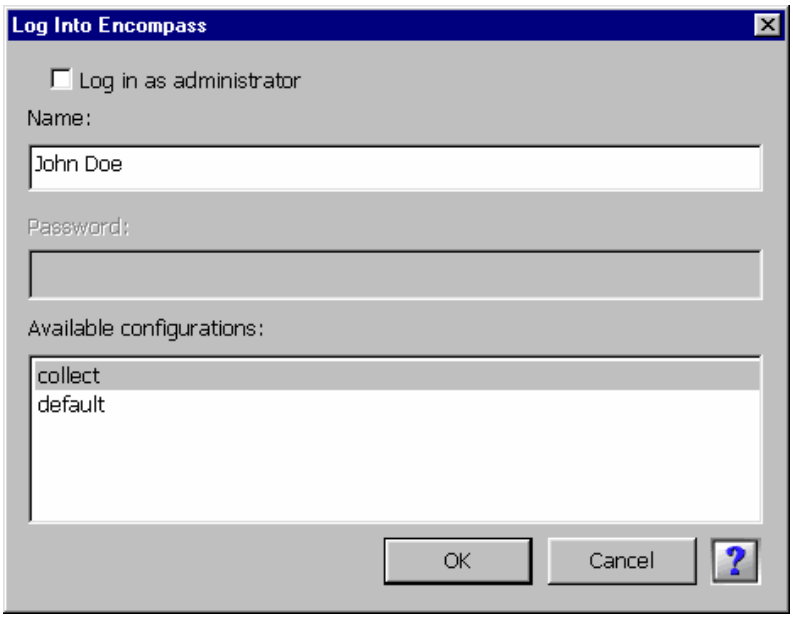
   Alternatively, you can click the Start button on the Windows taskbar, point to Programs (All Programs in Windows XP), point to the Thermo Scientific OMNIC folder, and then click the Encompass program.

   If you are not prompted to enter your name, the procedure is finished and you can now use the software. Otherwise, go to the next step.

3. **If you are prompted to log into Encompass, enter your user name and select a configuration or macro if any are listed.**

   Type your user name in the Name text box.

The appearance of this dialog box varies depending on how the software has been set up and which model spectrometer you have.



If you want to log in as the system administrator, turn on the Log In As Administrator check box. You must also enter the administrator's password in the Password text box. (The administrator is given access to software options that control how the system is used. See "Using System Manager" in the "Software Management" chapter for details.)

If the system has been set up to allow access only to certain configurations, they are listed in the Allowed Configurations box. Select the desired configuration by clicking it. See the "Software Management" chapter for information about configurations.

If the system has been set up to use macro mode, the available macros are listed in the Available Macros box (it appears instead of the Available Configurations box). Select the desired macro by clicking it. This macro will start when you choose OK to close the Log Into Encompass dialog box in the next step. See "Macro mode" in the "Software Management" chapter for more information about macro mode.

4. **Choose OK.**

   You can now use the software.

   If the system has been set to use macro mode, the macro you selected in step 3 starts running. Respond appropriately to any prompts that appear. (See the "Running a Macro" chapter of the *Encompass Macros User's Guide* for more information on running a macro.) When the macro is finished running, the Log Into Encompass dialog box reappears, allowing you to run another macro (see step 3). Another user or the administrator can also log in at this time.

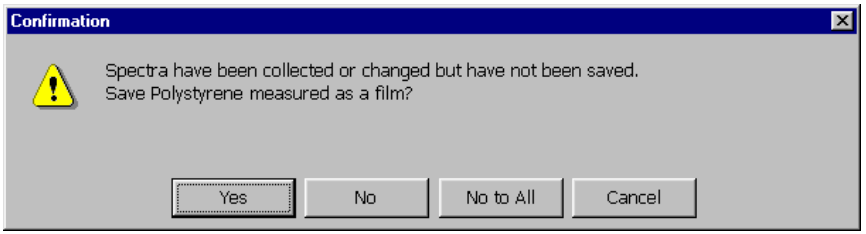
Collecting your first spectrum

If you are using the system for the first time and want to collect your first spectrum, read the "Collecting Spectra" chapter now. ▲

Exiting the software

If you have a Nicolet IR100, Encompass is exited when you turn off the spectrometer power.

If you have a Nicolet IR200, click the Exit button to exit the software. If you have collected or changed a displayed spectrum but have not yet saved it, the prompt shown below appears.

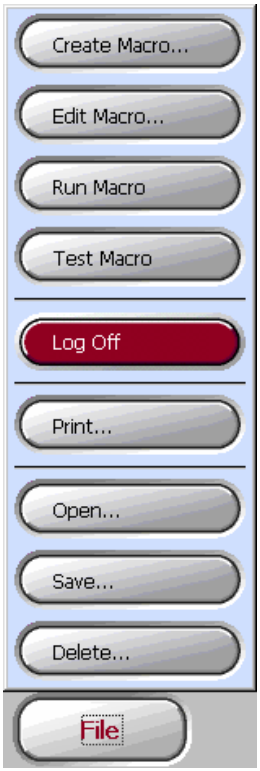


Note Since you cannot save a spectrum exported from a commercial library, this prompt does not appear for a commercial library spectrum. ▲

- If you want to save the spectrum, choose Yes. The Save As dialog box appears allowing you to save the spectrum. See “Saving a spectrum or report” in the “Opening and Saving Spectra and Reports” chapter if you need help.
- If you don’t want to save the spectrum, choose No (or No To All if you want to discard all of the collected or changed spectra that have not been saved).
- If you want to cancel the exit operation, choose Cancel.

Important If you want to save any results that you have added to a report, be sure to save the report before exiting Encompass. The report display will be cleared when you exit. See “About reports” in the “Using the Software Display” chapter and the “Opening and Saving Spectra and Reports” chapter for more information. ▲

Logging off Encompass



If you were required to log in (that is, enter your user name) when you started Encompass, use the Log Off command available through the File button to log off when you are finished using the software.

If you are the system administrator and have just set the system to require users to log in, you can also use the command to log off and display the log-in prompt. See “Using System Manager” in the “Software Management” chapter later in this manual for more information.

If you want to save any results that you have added to a report, be sure to save the report before logging off Encompass. The report display will be cleared when you log off. See “About reports” in the “Using the Software Display” chapter and the “Opening and Saving Spectra and Reports” chapter for more information.

Follow these instructions to log off Encompass:

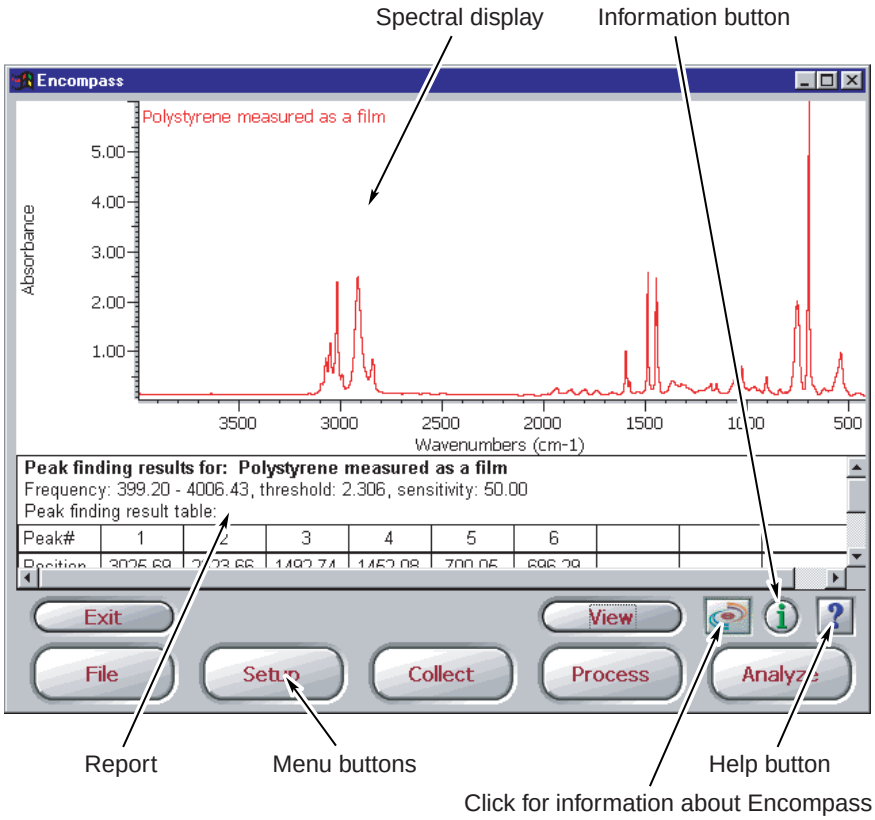
Click the File button and then choose Log Off from the menu.

The Log Into Encompass dialog box appears, and the system is ready for another user to log in. See “Starting the software” earlier in this chapter for information on logging into Encompass.

Using the Software Display

When Encompass starts, the window shown in the example below appears. It contains a spectral display for viewing spectra, plus buttons for performing operations and viewing information.

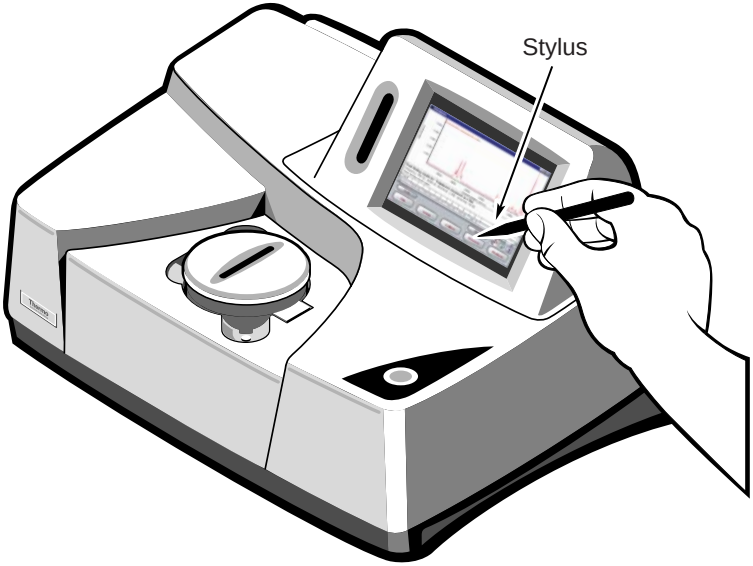
If your system has been set to use macro mode, some of the features shown are not available. See “Macro mode” in the “Software Management” chapter for details.



Depending on the operation you are performing, other features can appear in the window. For example, if you have a Nicolet IR100, a keyboard appears when you are entering text during some operations.

If you have a Nicolet IR200, the window has a title bar containing buttons for changing the size of the window and closing the window. Use these buttons just as you would in any Windows application. If the window is not maximized, you can also drag its borders and corners to change its size or drag its title bar to move it on the screen. See your Windows documentation if you need help using these features.

If you have a Nicolet IR100 with the optional touch screen display, the software responds when features are touched with one of the provided styluses. You can store a stylus in the groove at the top of the touch screen housing. Use the pointed end of the stylus as shown below to choose buttons, set options, enter text and perform other operations. See “Calibrating the touch screen” later in this chapter for information on calibrating the touch screen for proper operation.

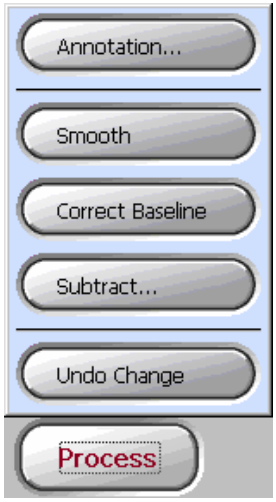


If you want to see information about Encompass, including the version number of the software, click the button bearing the Encompass logo. Choose Close when you are finished viewing the information.

The next sections explain how to use the software display features.

Using the menu buttons

Some of the buttons in the Encompass window are “menu buttons,” because a menu of related commands appears when you click the button. For example, when you click the Process button, a menu of commands related to data processing appears:



Commands are available only when they can be used. For example, the Subtract command is available only if two or more spectra are displayed.

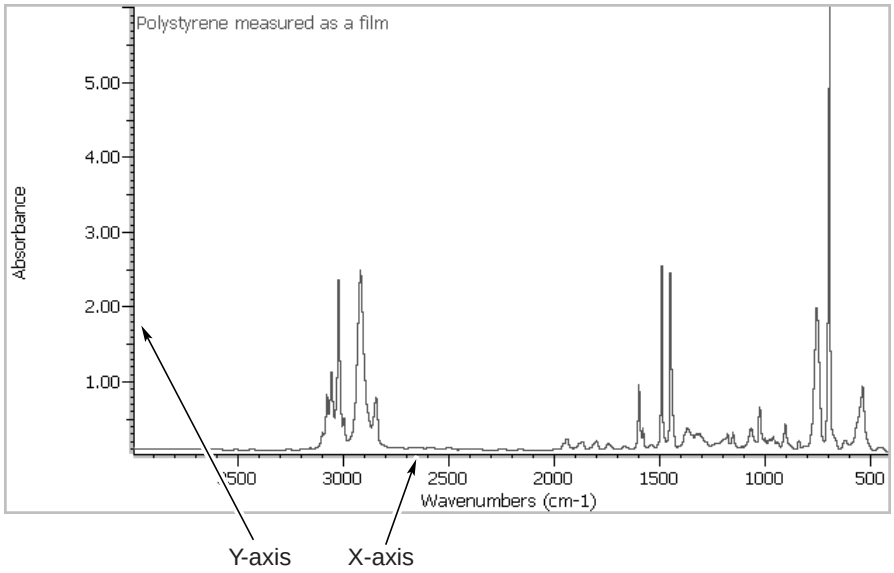
To choose a displayed command, click it.

When you choose some commands, a dialog box or other features appear. These are covered in the sections explaining the particular command later in this manual.

Note If your system has been set to use macro mode, the menu buttons are not available. Instead, you perform operations by running macros. See “Macro mode” in the “Software Management” chapter for more information. ▲

Using the spectral display

After you open or perform various operations on a spectrum, it appears in the spectral display. The display includes an X-axis and a Y-axis, with appropriate unit labels. (Multiple axes may appear depending on how you have set up the display. See “Overlaying or stacking spectra” in the “Software Management” chapter for details.)



You can select a displayed spectrum for an operation, clear a spectrum from the screen, or label features in a spectrum. These features are explained in the next sections.

You can also change the way spectra are displayed by setting the display options. These options are normally saved in a configuration that also includes options affecting data collection, library searches and printing. By opening a configuration, you can set the software for your preferences in one step. See “Setting the display options” and “Saving a configuration” in the “Software Management” chapter for more information.

Selecting a spectrum

Before you perform an operation on a displayed spectrum, select it by clicking it or its title (if displayed). The spectrum is then displayed in the color specified for the selected spectrum, typically red. See “Specifying colors for displaying spectra” in the “Software Management” chapter for more information.

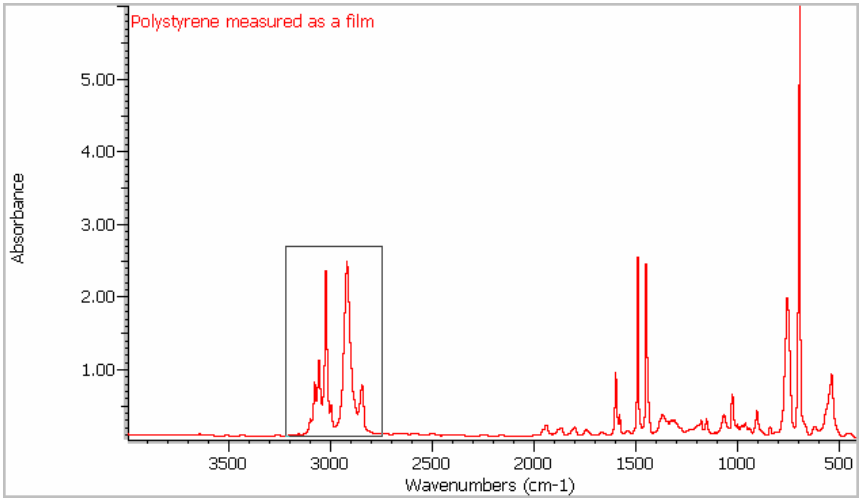
Zooming in on a spectrum

You can zoom in on a portion of a spectrum in the spectral display to see it better. Follow these steps:

1. **Draw a box around the area in the spectral display that you want to expand.**

   First point to a location for a corner of the box. Hold down the mouse button and drag the pointer across the screen to the desired location for the opposite corner. Then release the mouse button. (If you have a touch screen, use a stylus to draw a box on the screen.)

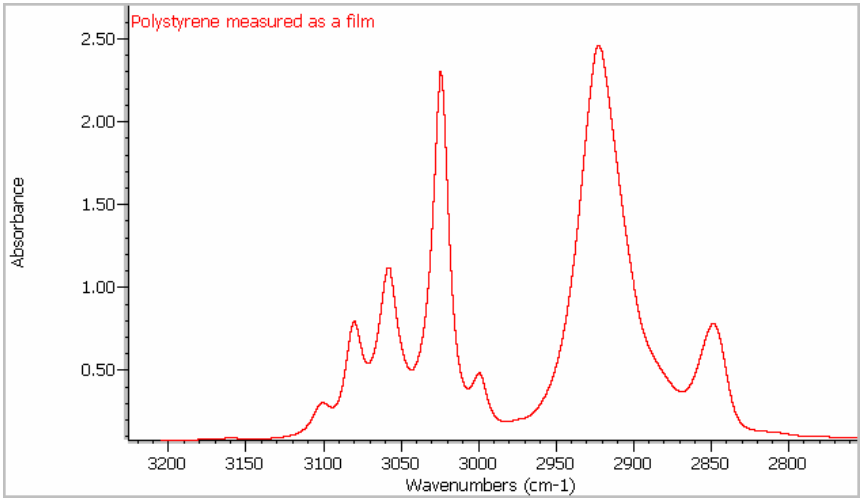
   Here is an example showing a drawn box:



2. **Click inside the box.**

The boxed portion of the spectrum expands to fill the spectral display.

If more than one spectrum is displayed, all are expanded in a similar manner.



You can restore the spectrum to its original size and position by using the Full Display command available through the View button (see the next section).

Zooming out

After you have zoomed in on a portion of a spectrum (see the preceding section), you can use the Full Display command available through the View button to zoom back out. The command displays all the open spectra using the spectral region specified by Start Frequency and End Frequency in the display options.

If Full Scale is selected in the display options, the Full Display command places the highest point of each spectrum at the top of the spectral display (or the top of the spectrum's pane if the spectra are stacked) and the lowest point of each spectrum on the X-axis.

If Common Scale is selected in the display options, the Full Display command displays all the spectra using the same Y-axis. The highest point among all the spectra is placed at the top of the spectral display (or the top of the spectrum's pane if the spectra are stacked), and the lowest point among all the spectra is placed on the X-axis.

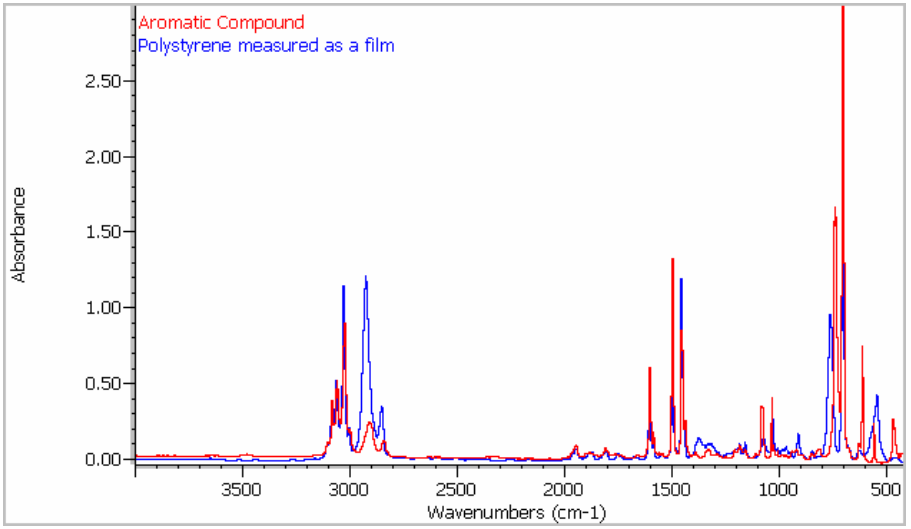
See "Setting the spectral region to display" and "Displaying spectra full scale and with a common scale" in the "Software Management" chapter for more information.

Follow these instructions to use the Full Display command:

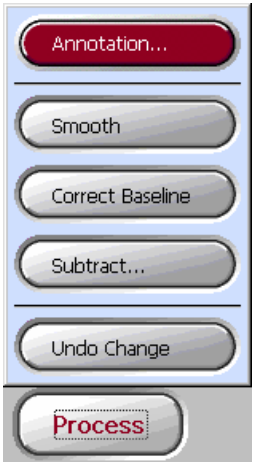
Click the View button and then choose Full Display from the menu.

The open spectra are displayed using the specified display limits.

Here is an example:



Labeling a spectrum



Use the Annotation command available through the Process button to label features in a spectrum. You can include the frequency location of a peak or any other information you want the label to show. You can also use the command to move or delete an existing label, including those added with Peak Height, Peak Area or Find Peaks available through the Analyze menu.

Labels you add will appear in the spectral display only if Show Annotations is selected in the display options. See “Displaying annotations” in the “Software Management” chapter for details.

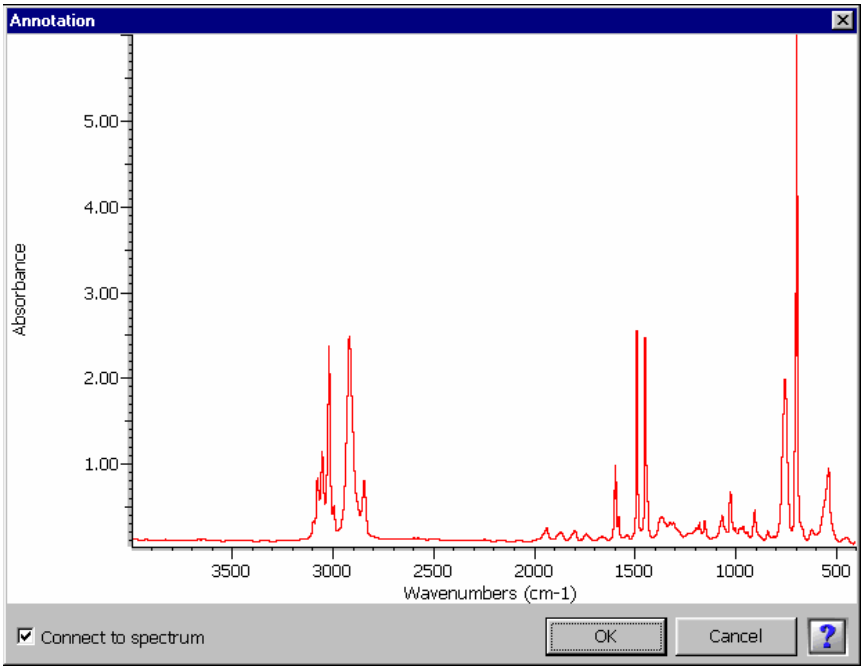
Follow these steps to label the selected spectrum:

1. **If desired, zoom in on the area around the peak or peaks you want to label.**

   It can be easier to label a small peak or a peak that is very close to others if you first zoom in on the area around it. See “Zooming in on a spectrum” in the “Using the Software Display” chapter earlier in this manual if you need help.

2. **Click the Process button and then choose Annotation from the menu.**

   A window appears showing the currently displayed portion of the selected spectrum:



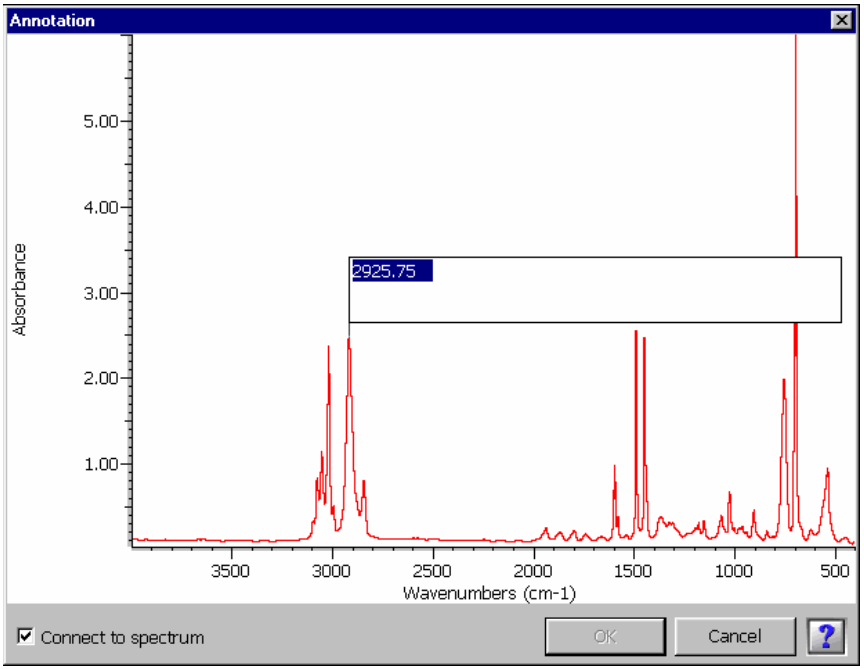
3. **If you don't want the label to be connected to the spectrum with a vertical line, turn off Connect To Spectrum.**

   Leave the option selected, or select it, if you want the label connected with a line.

4. **Click a location for the start of the label text.**

   Typically a location a little above the spectral feature of interest is used. (In a % transmittance spectrum a location a little below the feature is used.)

A box appears at that location showing the X value. Here is an example:



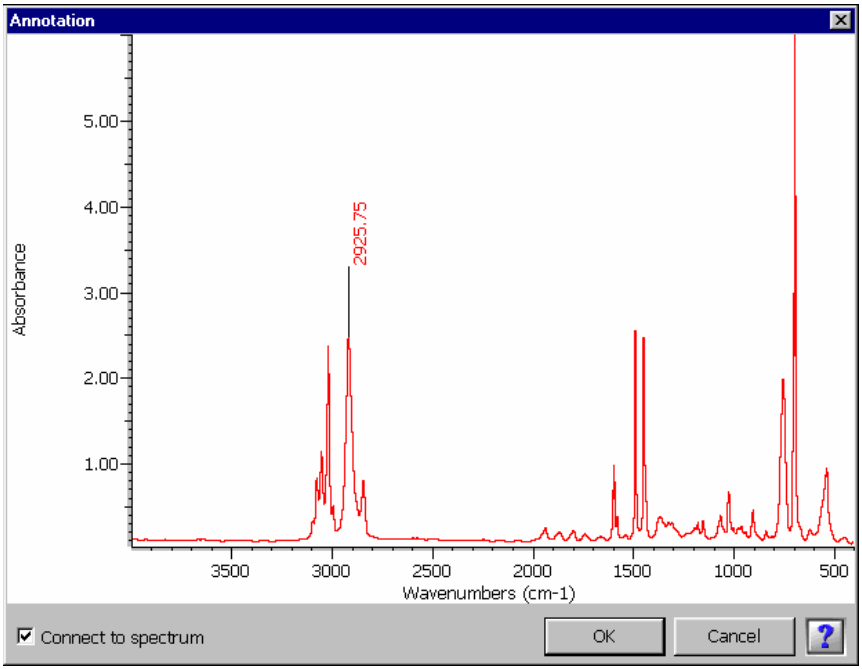
The text is selected to allow you to edit if desired.

5. **To accept the default text, click or press the Enter key (green arrow key on a Nicolet IR100 software keyboard). To change the text, type the desired text and then click or press Enter.**

   Try to keep your labels brief. If the text is too long to fit within the spectral display, the label will be truncated.

   If you delete all of the text, the label will be deleted when you click or press Enter.

The finished label is displayed perpendicular to the X-axis. Here is an example:



You can drag the label text (of any displayed label) to another location if desired.

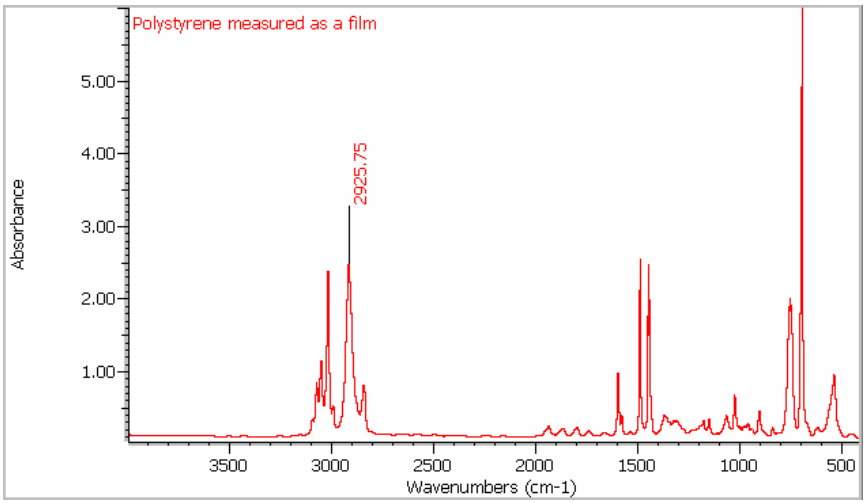
You can delete an existing label by clicking it, deleting all of the text and then clicking or pressing Enter.

To add another label, repeat steps 3 through 5.

6. **Choose OK.**

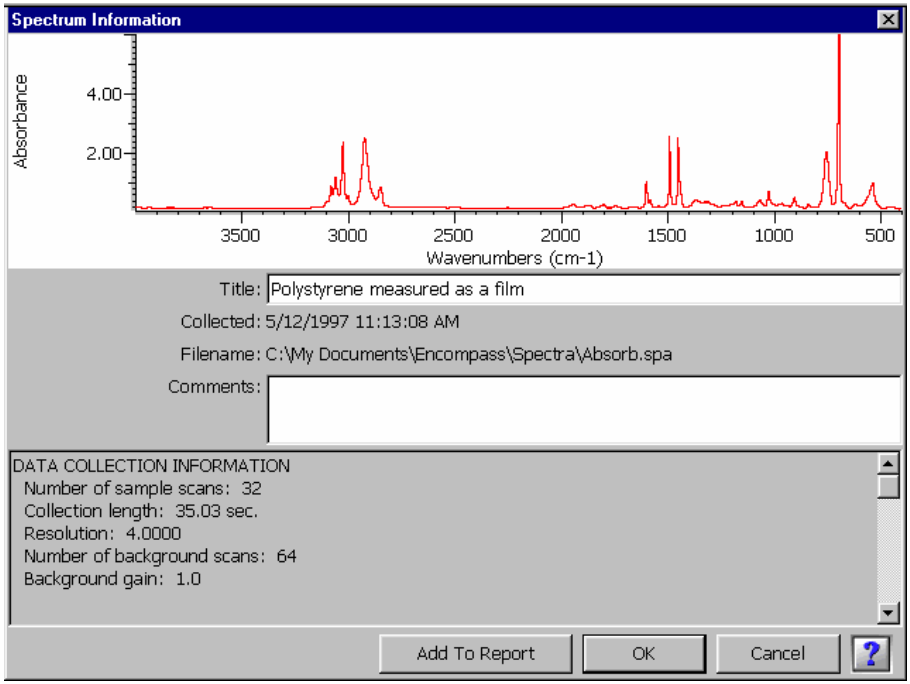
Choose Cancel if you want to end the procedure without keeping your changes.

The labels appear in the spectral display if Show Annotations is selected in the display options:



Viewing information about a spectrum

Use the Information button to see or enter information about the selected spectrum. Here is an example:



You can edit the title of the spectrum in the Title box, or enter or edit comments about the spectrum in the Comments box. If you have a Nicolet IR100, click inside the text box to display the software keyboard.

Below the title are the date the spectrum was collected and the filename of the spectrum.

Information about how the spectrum was collected and processed appears at the bottom of the window. Use the scroll bar at the right to bring information into view.

If you want to add the information to the report, choose Add To Report. See “About reports” later in this chapter for details about working with reports.

To specify the font for displaying text added to the report, set Font Name and Font Size in the print options. See “Setting the print options” in the “Software Management” chapter for details.

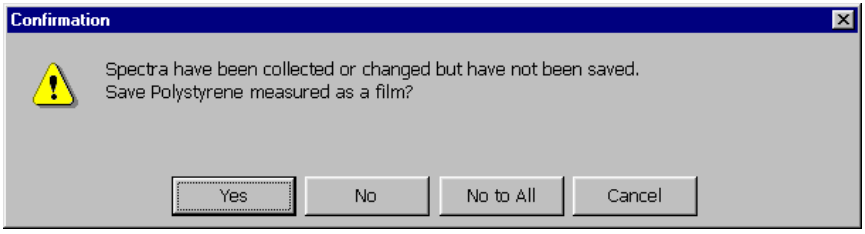
When you are finished viewing or entering information, choose OK, or choose Cancel to cancel your changes.

Clearing a spectrum

Use the Clear Spectrum command available through the View button to remove the selected spectrum from the spectral display. Follow these steps:

1. **Click the View button and then choose Clear Spectrum from the menu.**

   If you have collected or changed the spectrum but have not yet saved it, the prompt shown below appears. Otherwise, the spectrum is cleared and the procedure is finished.



Note Since you cannot save a spectrum exported from a commercial library, this prompt does not appear if you are clearing a commercial library spectrum. ▲

2. **If you want to save the spectrum, choose Yes. If you don't want to save it, choose No. If you want to cancel the clear operation, choose Cancel.**

   If you choose Yes, the Save As dialog box appears allowing you to save the spectrum. See "Saving a spectrum or report" in the "Opening and Saving Spectra and Reports" chapter if you need help. After you save the spectrum, it is cleared from the display, and the procedure is finished.

   If you choose No (or No To All), the spectrum is cleared and the procedure is finished.

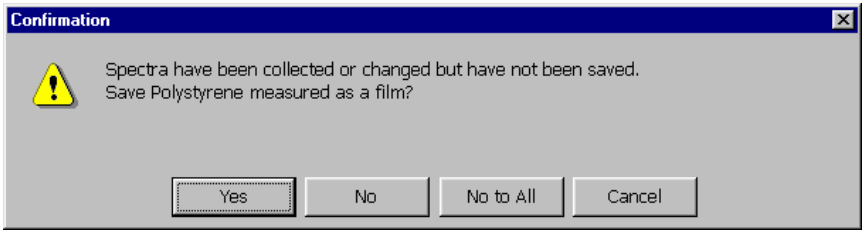
   If you choose Cancel, the spectrum remains in the spectral display, and the procedure is finished.

Clearing all the displayed spectra

Use the Clear All Spectra command available through the View button to remove all the spectra from the spectral display. Follow these steps:

1. **Click the View button and then choose Clear All Spectra from the menu.**

   If you have collected or changed any of the displayed spectra but have not yet saved them, the prompt shown below appears for the first of these spectra. Otherwise, the spectra are cleared and the procedure is finished.



Note Since you cannot save a spectrum exported from a commercial library, this prompt does not appear when you clear a commercial library spectrum. ▲

2. **If you want to save the indicated spectrum, choose Yes. If you don't want to save it, choose No; if you don't want to save it or any of the other spectra, choose No To All. If you want to cancel the clear operation, choose Cancel.**

   If you choose Yes, the Save As dialog box appears allowing you to save the spectrum. See "Saving a spectrum or report" in the "Opening and Saving Spectra and Reports" chapter if you need help. After you save the spectrum, it is cleared and the procedure continues with the next unsaved spectrum, if one exists. Respond appropriately each time the prompt appears.

   If you choose No, the spectrum is cleared and the procedure continues with the next unsaved spectrum, if one exists. Respond appropriately each time the prompt appears.

   If you choose No To All, the indicated spectrum and all the remaining spectra are cleared, and the procedure is finished.

   If you choose Cancel, the spectrum remains in the spectral display, and the procedure is finished.

Using the software keyboard

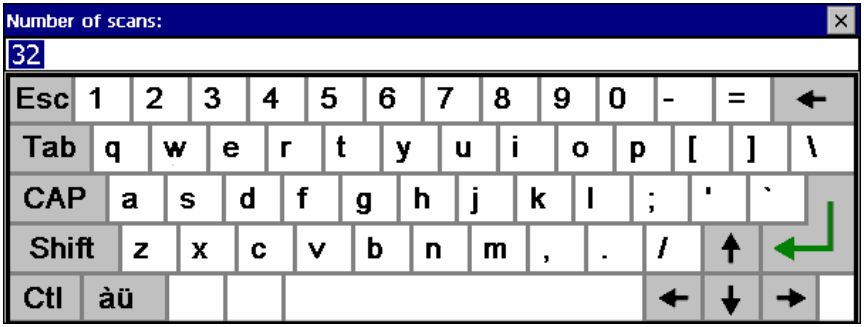
If you have a Nicolet IR100, a keyboard appears on the screen when you need to enter text for some operations. (If you have a Nicolet IR200, the software keyboard does not appear since your computer includes a keyboard for entering text.)

Note If you are using an external keyboard with a Nicolet IR100, the software keyboard does not appear. See "Using an external keyboard with a Nicolet IR100" in the "Welcome" chapter for more information. ▲

Follow these steps to display and use the software keyboard:

1. **Click in the text box in which you want to enter text.**

   The software keyboard appears. Here is an example:



Note The keyboard displayed by some features may have a somewhat different appearance, but it is used in essentially the same way. ▲

   The description at the top of the keyboard matches the name of the feature for which you are entering text.

2. **Type the needed text by clicking characters on the keyboard.**

   If you make a mistake, you can use the left arrow key near the upper-right corner of the keyboard to delete characters you have typed.

   To display a set of keys for typing international symbols and letters, click the key labeled “àü.” To return to the standard set of keys, click the “àü” key again.

3. **When you are finished, click the Enter key, the key that shows a green arrow.**

   The keyboard is removed from the screen and the text you typed appears in the text box.

   If you want to cancel the operation and not use the text you typed, click the Esc key or the Close button (labeled “X”) in the upper-right corner of the keyboard window.

Note If you click the Enter key and then decide to change the text you just entered, you must first do either of two things before you can display and use the keyboard again for that text box: You can use another feature in the dialog box or window and then click in the text box, or you can display the keyboard by clicking in another text box, close the keyboard, and then click in the text box whose text you want to change. ▲

About reports

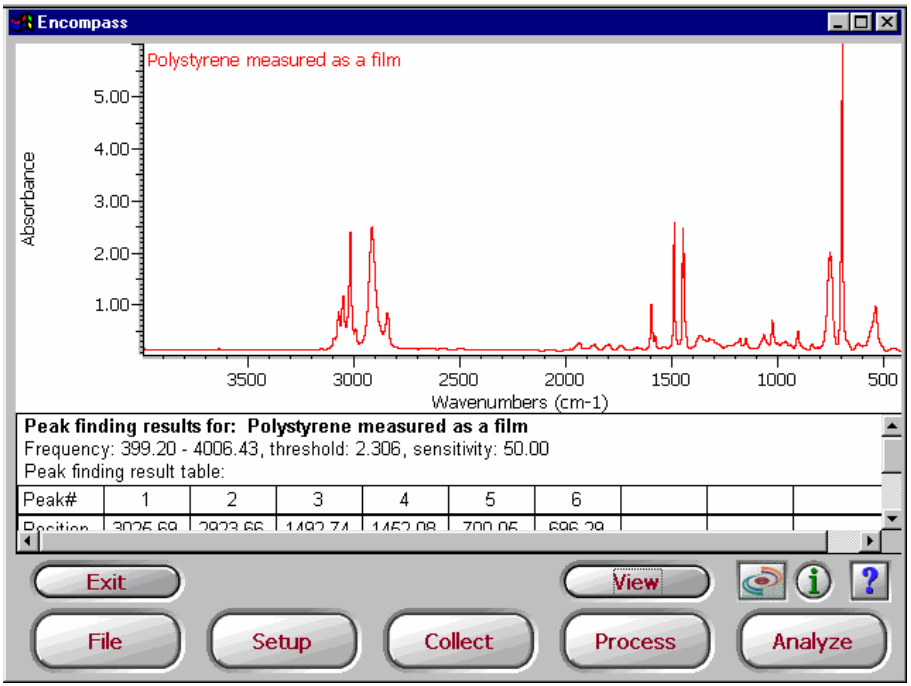
After you perform any of the following operations with commands available through the Analyze button, you can click the OK button to add the results of the operation to a report that you can display below the spectral display (see the next section for instructions).

- Find peaks with the Find Peaks command.
- Measure the height of a peak with the Peak Height command.
- Measure the area of a peak with the Peak Area command.
- Search a spectral library with the Search Library command.
- Compare spectra with the Compare command.

You can also add information about a spectrum to the report by choosing Add To Report in the Spectrum Information window. See "Viewing information about a spectrum" earlier in this chapter for details.

If you have a Nicolet IR100 and have purchased additional spectral libraries from us on a flash memory card, you can display a list of the libraries contained on the card in the report. See "Viewing a list of the libraries contained on a flash memory card" in the "Software Management" chapter for details.

Here is an example showing a report displayed in the Encompass window:



Each time you perform an operation and add its results to the report, they appear at the end. When needed, a scroll bar at the right side of the report lets you scroll results into view.

To specify the font for displaying text added to the report, set Font Name and Font Size in the print options. See “Setting the print options” in the “Software Management” chapter for details.

The next sections explain the things you can do with reports.

Displaying or hiding the report

If the report is not currently displayed, you can display it by clicking the View button and choosing Show Report.

The name of the command then changes to Hide Report. Click the View button and choose Hide Report if you want to remove the report from the display.

Clearing the report

To clear the information from the report, click the View button and then choose Clear Report.

All of the results in the report will be deleted, so be sure you want to clear the report before choosing the command.

Printing the report

You can use the Print command available through the File button to print the report on paper. To set the options that control how the report is printed, use the Print Options command available through the Setup button. See the “Printing Spectra and Reports” chapter and “Setting the print options” in the “Software Management” chapter for details.

Saving and opening reports

You can use the Save command available through the File button to save the report (in plain text format) in a file that can be opened later. Use the Open command available through the File button to open a saved report. If you open a report, any results you add will be added to that report. To delete a saved report, use the Delete command available through the File button.

Important If you don't save the report, the information it contains will be lost when you exit or log off Encompass. ▲

For more information see "Opening a spectrum or report" and "Saving a spectrum or report" in the "Opening and Saving Spectra and Reports" chapter, and "Deleting a file or folder" in the "Software Management" chapter.

Note Since reports are saved as text files (having the extension .TXT), you can open and edit a saved report using Notepad, WordPad, Microsoft® Word or other programs that open text files. Since a text file does not contain formatting information, a report you open in another program may look different from how it looked in the Encompass window. ▲

Calibrating the touch screen

If you have a Nicolet IR100 with a touch screen, it was calibrated for accuracy at our factory. If you ever notice that the software does not respond as expected when you touch a feature—for example, you find that you must touch a short distance away from a button to make it respond—the screen should be recalibrated. Follow these steps:

1. **Touch the Setup button and then choose System Manager from the menu.**

   System Manager appears. For more information about System Manager, see “Using System Manager” in the “Software Management” chapter.

2. **Touch the Calibrate Screen button and then follow the instructions that appear on the screen.**

3. **When the calibration is finished, choose OK to close System Manager.**

Software Management

This chapter covers software management, an aspect of using Encompass normally handled by a system administrator. If you are a user who is not responsible for software management tasks, you can skip this chapter.

Encompass software management can involve three main parts:

Software security – This is used by the system administrator to control who uses the software. Through System Manager, the administrator can require that users log in by entering a user name before using Encompass.

Note When you first use the software, no security is set up. Use System Manager available through the Setup button if you want to set up software security. ▲

Configurations – These contain option settings that determine how spectra are displayed and how other software features operate. Setting up and saving different configurations saves the time it would take to set many individual options each time different settings were needed for a procedure.

The system administrator can allow users the freedom to set options and use any saved configuration, or limit users to particular configurations, without the ability to change option settings.

Macro mode – If you purchased Encompass Macros, macro mode can be selected by the system administrator to give users access only to macros that perform approved tasks, rather than having access to the menu buttons and commands.

Note Encompass Macros lets you create, edit, run and test macros when the software is not in macro mode. See “Using macros” later in this chapter and the *Encompass Macros User’s Guide* for more information. ▲

The next sections explain how to perform these software management tasks:

- Set the options that affect the spectral display, data collection, library searches and printing. See “Working with configurations.”
- Open and save configurations. See “Opening a configuration” and “Saving a configuration.”
- Set up software security, including control over which configurations or macros are available to users. See “Using System Manager.”
- Use macros. See “Using macros.”

In addition, this chapter explains how to perform these other tasks related to software management:

- Delete a file containing a spectrum, report, configuration or macro, or a folder (on a Nicolet IR100 only). See “Deleting a file or folder.”
- Set up networking for a Nicolet IR100. See “Setting up networking for a Nicolet IR100.”

If you have a Nicolet IR100 and wish to use flash memory cards to store files, be sure to read the last section of the chapter, “Using flash memory cards.”

Important We recommend that you routinely back up your spectral data, macros and other important files. Be sure to do this before you install a new version of Encompass. Depending on your system, you can use flash memory cards, a network or other types of storage media for this. When you are saving an important file, consider saving an extra copy in a location other than the internal flash memory or hard disk. To back up files that you saved earlier, open them and then save them in an external location. See “Backing up a macro” in the “Editing a Macro” chapter of the *Encompass Macros User’s Guide* for instructions for backing up macros. ▲

Working with configurations

Configurations contain options set using the following commands available through the Setup button:

- Display Options
- Collect Options
- Search Options
- Print Options

The options determine how spectra are displayed and how other software features operate. The next sections explain how to set the options and how to open and save configurations that contain your settings.

For information on controlling user access to configurations or to the options commands, see “Using System Manager” later in this chapter.

Setting the display options

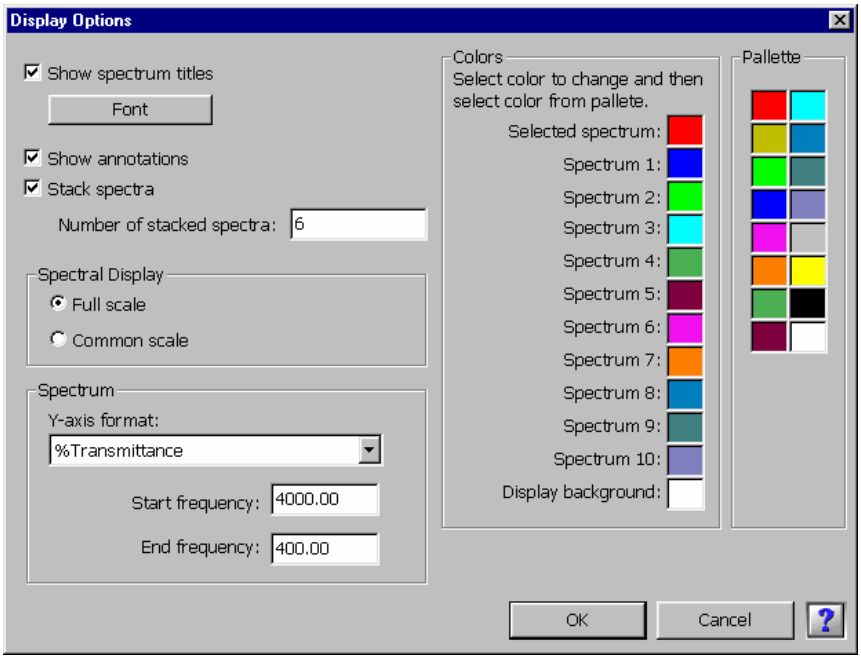
Use the Display Options command available through the Setup button to set the options that determine how spectra are displayed.

If the display option settings you need are already saved in a configuration, you can set the software in one step by opening the configuration. After you use Display Options to set the software for your preferences, you can save your settings in a configuration that can be opened later. See “Opening a configuration” and “Saving a configuration” later in this chapter for details.

Follow these steps to set the display options:

1. **Click the Setup button and then choose Display Options from the menu.**

   The display options appear:



2. **Set the options as desired.**

   See the next sections for detailed instructions.

3. **Choose OK.**

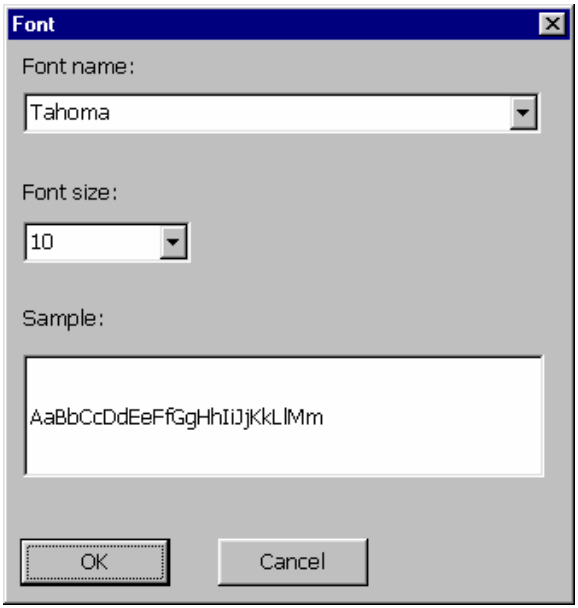
Displaying the titles of spectra

Turn on Show Spectrum Titles if you want to display the titles of all the open spectra, with each title shown in the same color as the corresponding spectrum.

After you turn on Show Spectrum Titles, you can specify a font for displaying the titles. Follow these steps:

1. **Click the Font button.**

   The Font dialog box appears:



2. **Select a font from the Font Name drop-down list box.**

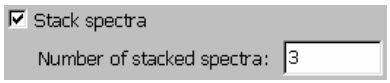
3. **Select a font size from the Font Size drop-down list box.**

4. **Choose OK.**

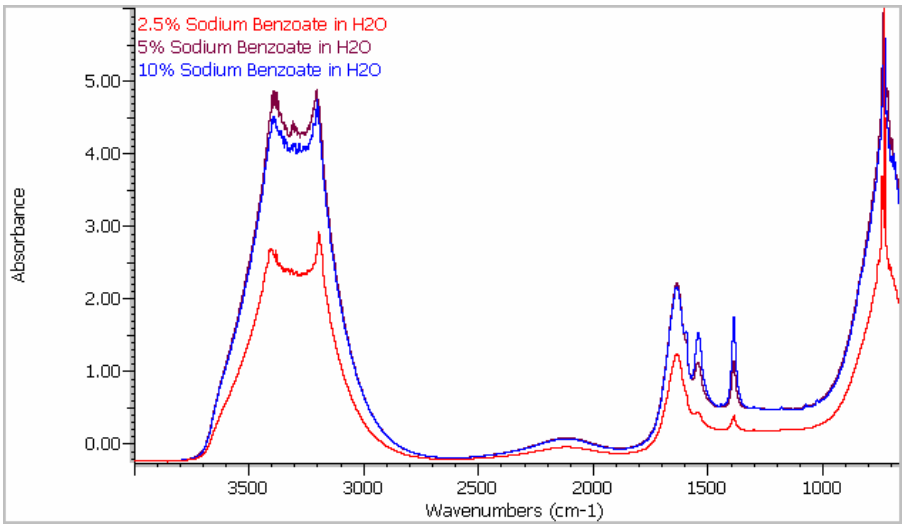
Displaying annotations

Turn on Show Annotations if you want spectra to be displayed with any annotations you have added. These annotations include those added with the Annotation command available through the Process button or with the Peak Height, Peak Area or Find Peaks commands available through the Analyze button. See “Labeling a spectrum” in the “Using the Software Display” chapter and “Measuring the height of a peak,” “Measuring the area of a peak” and “Find peaks” in the “Analyzing Spectra” chapter for more information.

Overlaying or stacking spectra

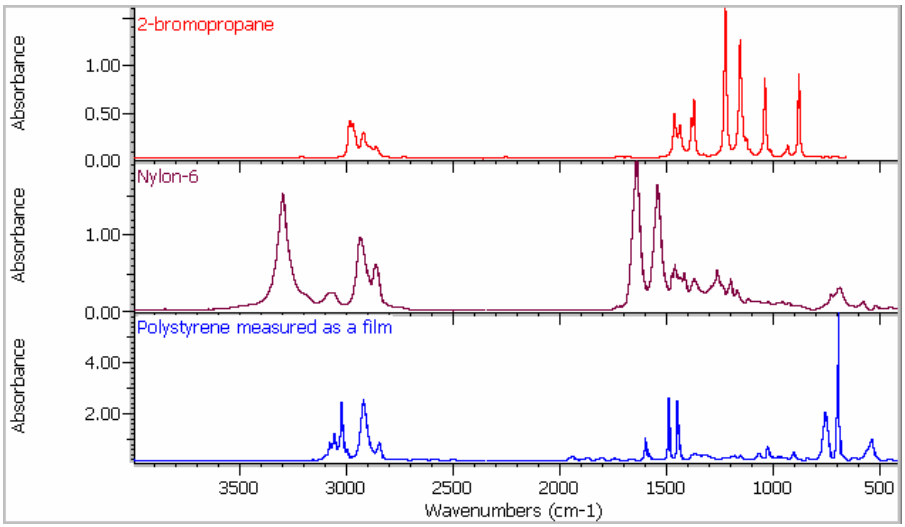


You can overlay spectra in the spectral display or “stack” them so that they appear above one another. Overlaying spectra makes it easy to see differences in their spectral features.



Overlaid spectra

Stacking spectra in their own “panes” is useful when you are comparing spectra that are significantly different.

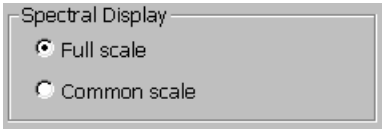


Stacked spectra

If you want to stack spectra, select Stack Spectra. Type the maximum number of spectra you want visible at one time in the Number Of Stacked Spectra text box. If you have a Nicolet IR100, click inside the text box to display the software keyboard. If more spectra are open than can be displayed at one time, a scroll bar appears at the right side of the spectral display so that you can scroll spectra into view.

If you want to overlay spectra, turn off Stack Spectra.

Displaying spectra full scale or with a common scale



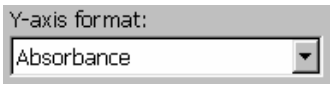
Specify the type of scale to use for displaying spectra by selecting Full Scale or Common Scale in the Spectral Display box.

If you select Full Scale, the spectral region specified by the Start Frequency and End Frequency text boxes in the Spectrum box is displayed, with the highest point of each spectrum at the top of the spectral display (or the top of the spectrum's pane if the spectra are stacked) and the lowest point on the X-axis. See "Specifying the spectral region to display" later in this chapter for information about setting the frequencies.

Note These display limits are also used if you later zoom in a portion of a spectrum and then use the Full Scale command available through the View button to zoom out. See "Zooming in on a spectrum" and "Zooming out" in the "Using the Software Display" chapter for more information. ▲

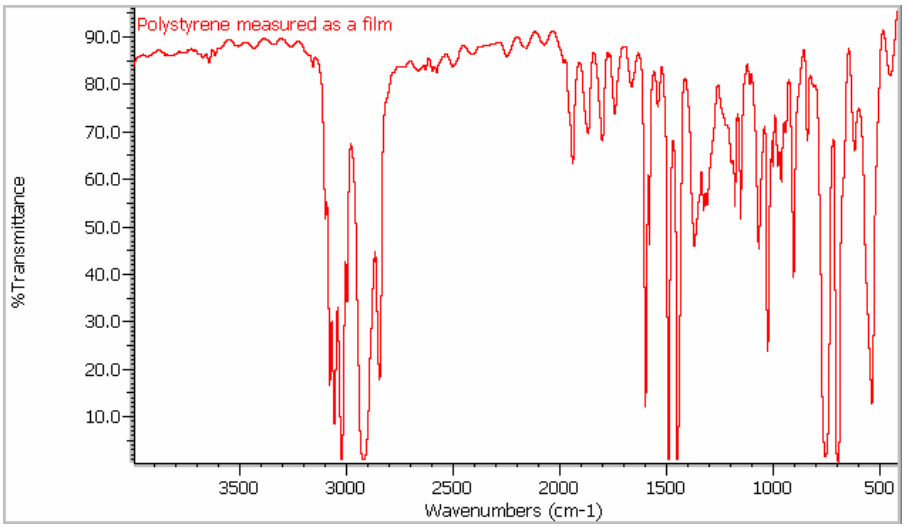
If you select Common Scale, all the spectra are displayed using the spectral region specified by the Start Frequency and End Frequency text boxes and with the same Y-axis scale. (The scale is adjusted so that all the peaks in all the spectra are visible.) This makes it easy to compare the relative intensities of peaks.

Displaying spectra in % transmittance or absorbance



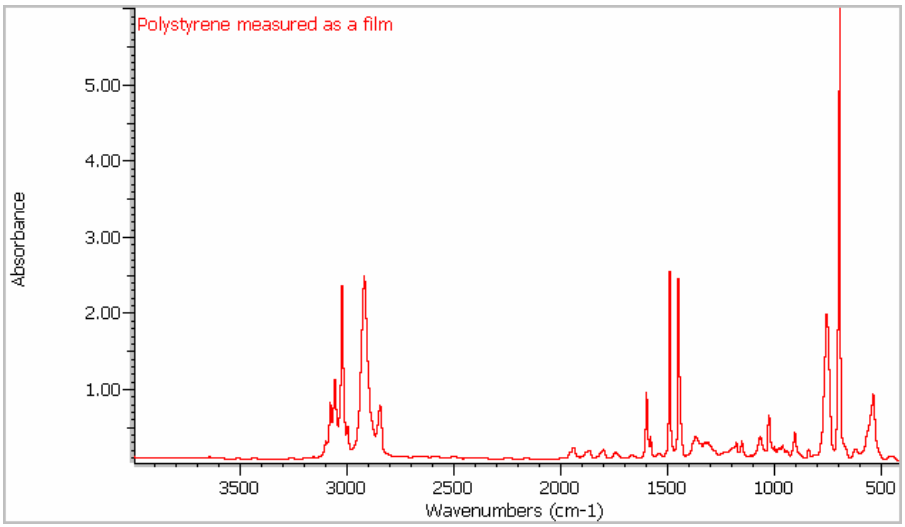
Use Y-Axis Format to specify the Y-axis units for displaying sample spectra. Click the down arrow button to display a list of available units, and then click the desired units.

Percent transmittance units show the relative amount of infrared energy transmitted through a sample. Here is an example:



Spectrum in % transmittance

Absorbance units show the amount of infrared energy absorbed by a sample. Here is an example:



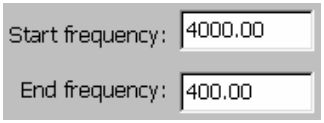
Spectrum in absorbance

You should normally display spectra in absorbance before performing these tasks:

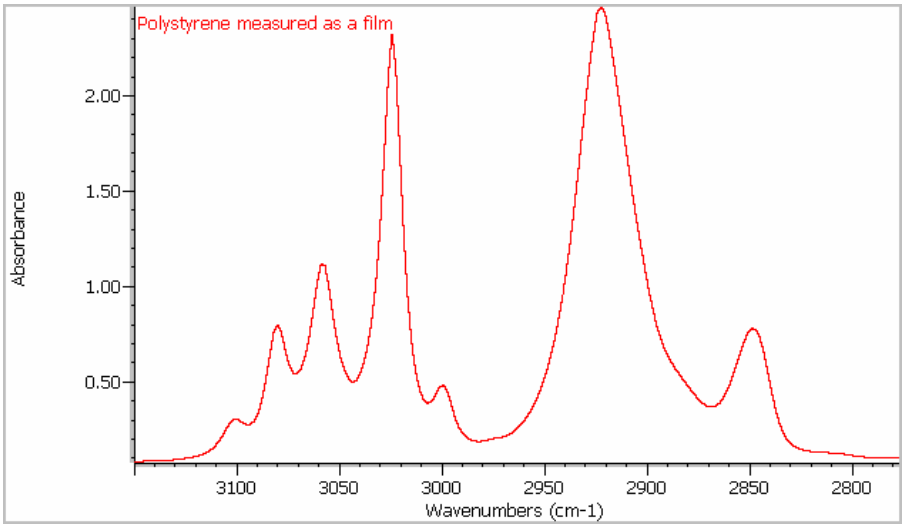
- Subtracting one spectrum from another.
- Correcting the baseline of a spectrum.
- Measuring the area of a peak.

Note Data displayed as an interferogram (with the Y-axis in volts and the X-axis in data points) cannot be converted to absorbance or % transmittance with Y-Axis Format. Interferograms are normally used only for maintenance and service procedures. ▲

Specifying the spectral region to display



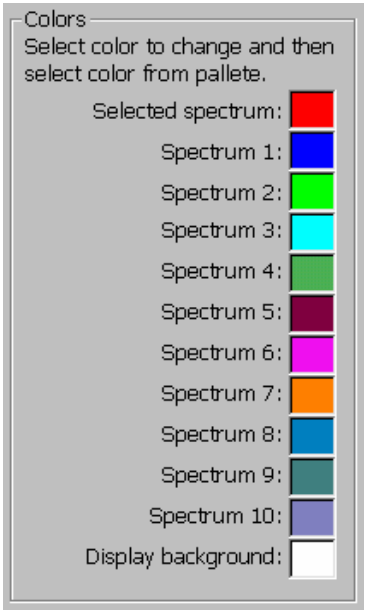
You can display spectra across their entire X-axis range or display only a particular spectral region. A spectral region is a portion of a spectrum that is between two specified X-axis values. A displayed region fills the spectral display, making spectral features larger and easier to see. Here is an example:



To specify the spectral region to display, type the starting and ending frequencies (X values) in the Start Frequency and End Frequency text boxes. If you have a Nicolet IR100, click inside the text box to display the software keyboard.

You can change the displayed spectral region by zooming in on an area within the spectral display or by using the Full Display command available through the View button. See “Zooming in on a spectrum” and “Zooming out” in the “Using the Software Display” chapter for details.

Specifying colors for displaying spectra



Displaying spectra in different colors makes them easier to see, especially when they are overlaid. The Colors box shows the colors currently selected for displaying the selected spectrum, spectra that are not selected, and the background of the spectral display.

The color of the selected spectrum is important, since it indicates which of the displayed spectra will be affected by operations you perform. Typically red is used for this.

Spectra that are not selected are displayed using the other colors, in the order shown as spectra are added to the display. After a spectrum is displayed using the last color (Spectrum 10), the assignment of colors starts again with the first color (Spectrum 1). The maximum number of spectra that can be displayed at one time is ten.

If you want to change a color, follow these steps:

1. **Click the color in the Colors box that you want to change.**

2. **Click the desired color in the palette of available colors.**

The color of the spectrum or display background changes to the color you selected.

Setting the data collection options

Use the Collect Options command available through the Setup button to set the options that control how spectra are collected.

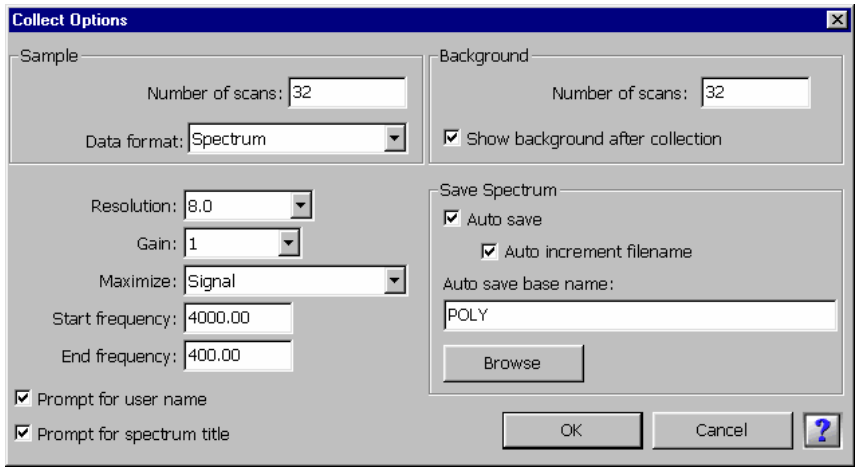
If the data collection option settings you need are already saved in a configuration, you can set the software in one step by opening the configuration. After you use Collect Options to set the software for your preferences, you can save your settings in a configuration that can be opened later. See “Opening a configuration” and “Saving a configuration” later in this chapter for details.

After you set the options, you can use the Background and Sample commands available through the Collect button to collect spectra. See “Collecting a background” and “Collecting a sample spectrum” in the “Collecting Spectra” chapter for details.

Follow these steps to set the data collection options:

1. **Click the Setup button and then choose Collect Options from the menu.**

   The data collection options appear:



2. **Set the options as desired.**

   See the next sections for detailed instructions.

3. **Choose OK.**

Setting the number of scans

Use Number Of Scans in the Sample box and Background box to specify the number of scans to collect during sample and background data collections, respectively. A single scan produces one interferogram. (An interferogram is the collected data before it is processed into a spectrum.) In a typical experiment 32 scans are performed. (Multiple scans are “coadded” to produce one interferogram.)

Type the desired value in the Number Of Scans text box. If you have a Nicolet IR100, click inside the text box to display the software keyboard.

Increasing the number of scans reduces the noise level and increases the sensitivity.

Specifying the format of the collected data

Use Data Format in the Sample box to specify the format of the collected data. Click the down arrow button to display a list of available settings, and then click the desired setting.

- If you select Spectrum, the data will be processed into a sample spectrum or background spectrum, depending on which type of spectrum you collect.

In Encompass a sample spectrum can be displayed with the Y-axis in absorbance units or % transmittance units; the X-axis is always in wavenumbers. You can convert an absorbance spectrum to % transmittance, and vice versa, by using the Display Options command available through the Setup button. See “Displaying spectra in absorbance or % transmittance” earlier in this chapter for more information, including examples.

- If you select Interferogram, the collected data (the interferogram) will not be processed into a spectrum. When you display an interferogram, the Y-axis is in volts and the X-axis is in data points. Interferograms are normally used only for maintenance and service procedures.

Displaying the background after it is collected

Turn on Show Background After Collection if you want background spectra to appear in the spectral display after they are collected. Regardless of whether a collected background is displayed, it is placed in memory so that it can be used to ratio sample spectra.

Setting the resolution

Use the Resolution option to set 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.

Set the resolution only as high as needed to differentiate peaks of interest and give good search results. Setting the resolution higher than required 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 or memory that is required to save the data.

Typically resolutions of 8 or 4 wavenumbers are used for solid and liquid samples. You must collect your sample and background spectra using the same resolution.

To set the resolution, click the down arrow button to display a list of available settings, and then click the desired setting.

Setting the signal gain

Use the Gain option to set the signal gain for sample and background data collection. The available settings are 1 and 4. The gain determines how much the detector signal is amplified electronically, making it larger relative to the level of electronic noise. Amplifying the signal—by setting Gain to 4—can be helpful when the signal is weak, such as when you use an ATR sampling accessory. Gain is normally set to 1 when an accessory is not being used.

To set the gain, click the down arrow button to display a list of the available settings (1 and 4), and then click the desired setting.

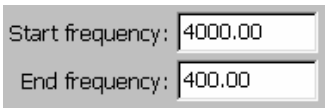
Important Do not use a setting of 4 if "clipping" of the signal occurs. A clipped signal appears as a flattened interferogram peak at +10 or -10 volts in the Diagnostics window. See the "Diagnostics" chapter for more information. ▲

Maximizing the detector signal or the resolution

Use the Maximize option to specify whether to maximize the detector signal or the resolution. Normally you should use the Signal setting. Select Resolution only if the resolution needs to be 1.0 wavenumber or better to resolve the peaks in your sample spectra.

To set this option, click the down arrow button to display a list of available settings, and then click the desired setting.

Specifying the spectral range



Specify the spectral range (X-axis range) of the data you will collect by typing starting and ending X values in the Start Frequency and End Frequency text boxes. If you have a Nicolet IR100, click inside the text box to display the software keyboard. The starting value should be larger than the ending value to reflect the way spectra are normally displayed when the X-axis is in wavenumbers.

Typically FT-IR spectra are collected using the entire mid-infrared range, 4,000 to 400 wavenumbers. You can set the system to collect data in a smaller range if you are interested in just a particular spectral region or are using an ATR accessory with a limited spectral range. Using a smaller range does not decrease the time needed to collect spectra, but it does reduce the amount of disk space required to save spectra.

Prompting for a user name

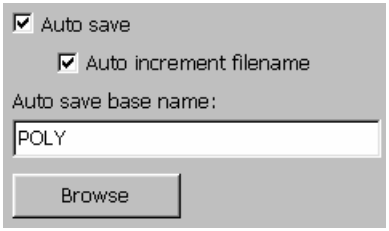
If you want to be prompted to enter a user name during data collection, turn on Prompt For User Name. If you later select the collected spectrum and click the Information button, the user name will appear in the "DATA PROCESSING HISTORY" section in the Spectrum Information window. See "Viewing information about a spectrum" in the "Using the Software Display" chapter for details.

Prompting for a spectrum title

If you want to be prompted to enter a title for the spectrum being collected, turn on Prompt For Spectrum Title. The title will appear in the spectral display when you display the spectrum if Show Spectrum Titles is selected in the display options. You will be able to change the title later if desired by using the Information button. See "Displaying the titles of spectra" and "Viewing information about a spectrum" in the "Using the Software Display" chapter for more information.

If Prompt For Spectrum Title is turned off, collected spectra will be titled with the current date and time. If a base name is entered in the Auto Save Base Name text box (see the next section), the base name will appear after the date and time.

Saving collected spectra automatically



If you want spectra you collect to be saved automatically after collection, turn on Auto Save. Then type the desired filename (without the extension) in the Auto Save Base Name text box, or use the Browse button to locate and select a file whose name you want to use (the existing file will be overwritten). (If you have a Nicolet IR100, click inside the text box to display the software keyboard for typing a filename.) If Prompt For Spectrum Title is turned off (see the preceding section), the name you specify will appear after the date and time in the spectrum title.

If you want the spectra saved in a location other than the default directory (Encompass\Spectra), type the pathname of the location or use the Browse button to specify a path. You can use this technique to save spectra in a network location, or on a flash memory card (on a Nicolet IR100 only).

Important If you have a Nicolet IR100, save spectra only in directories within the Encompass, Storage Card or Network directories (if present). Spectra saved in other directories will be lost when you turn off the spectrometer power. See “Specifying a network path for opening and saving spectra or reports” later in this chapter for more information on saving spectra and reports on a network. ▲

If Auto Increment Filename is off, each time you collect a spectrum, it will be saved automatically using the specified filename, overwriting any previously saved file having that name.

To prevent the overwriting of automatically saved files, turn on Auto Increment Filename. This appends a four-digit number to the base name. Each time you collect a spectrum, the number increases by one when the file is saved. For example, if the base name is “POLY,” a series of four automatically saved spectra will have these filenames:

POLY0000.SPA
POLY0001.SPA
POLY0002.SPA
POLY0003.SPA

If have a Nicolet IR100 and want the spectra saved on a flash memory card, be sure to install the card in the flash memory card slot on the front of the spectrometer before you begin collecting spectra.

Important Flash memory cards are sensitive to static electricity. When handling them, always follow the precautions given in “Using flash memory cards” later in this chapter. ▲

Setting the library search options

Use the Search Options command available through the Setup button to set the options that determine how library searches are performed.

If the search option settings you need are already saved in a configuration, you can set the software in one step by opening the configuration. After you use Search Options to set the software for your preferences, you can save your settings in a configuration that can be opened later. See “Opening a configuration” and “Saving a configuration” later in this chapter for details.

After you set the options, you can use the Search Library command available through the Analyze button to perform a search. See “Searching a spectral library” in the “Analyzing Spectra” chapter for details.

Follow these steps to set up a library search:

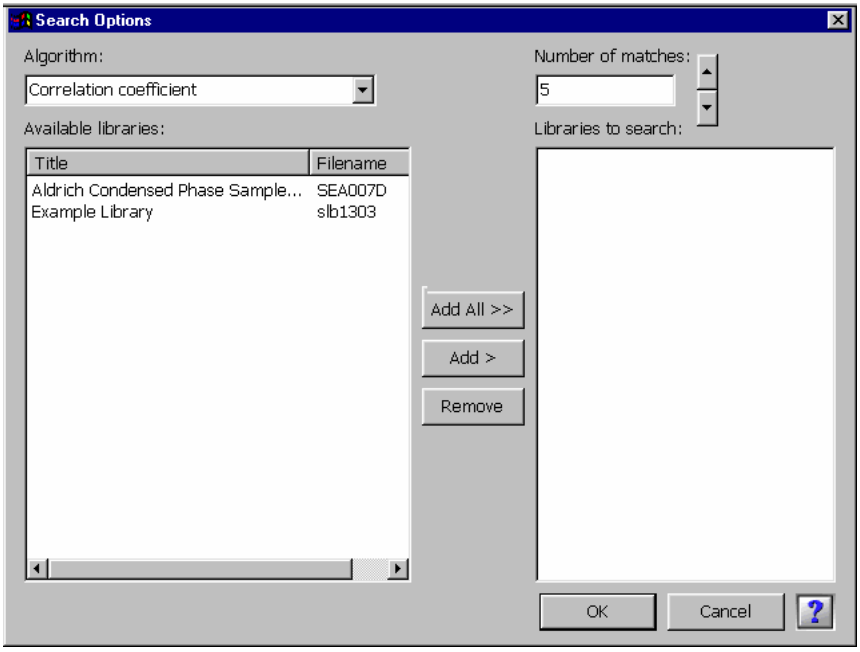
1. **If you have a Nicolet IR100 and the libraries you want to search are on a flash memory card, insert the card into the flash memory card slot on the front of the spectrometer.**

Important Flash memory cards are sensitive to static electricity. When handling them, always follow the precautions given in “Using flash memory cards” later in this chapter. ▲

   See “Using flash memory cards” later in this chapter for an illustration showing how to insert the card.

2. **Click the Setup button and then choose Search Options from the menu.**

   The library search options appear. Here is an example:



3. **Set the options as desired.**

   See the next sections for detailed instructions.

4. **Choose OK.**

Specifying the search algorithm

Use the Algorithm option to specify a search algorithm. It determines how a spectral search is carried out mathematically. Two algorithms are available:

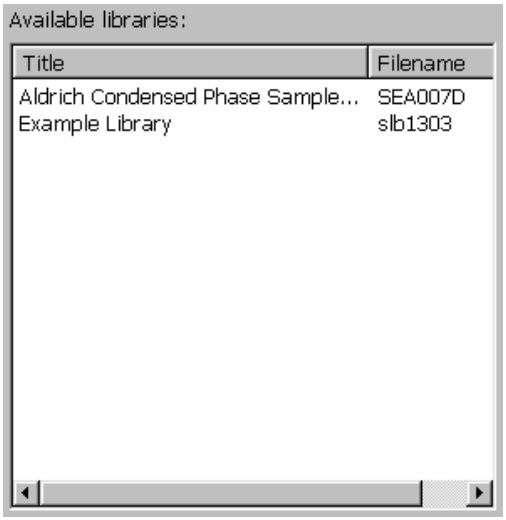
The **correlation coefficient** algorithm is recommended for most applications. It normally gives the best results when few of the spectra in the library are very similar to the sample spectrum. The algorithm also removes any effect of offset in the unknown spectrum, thus eliminating the effects of baseline variation.

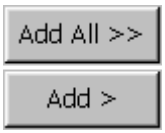
The **Euclidean distance** algorithm gives the best results when you are searching a library that contains a number of spectra that are very similar to the sample spectrum. The algorithm is also less sensitive than the correlation coefficient algorithm to noise. This makes the Euclidean distance algorithm the better choice when you are searching noisy spectra.

To select an algorithm, click the down arrow button to display a list of available algorithms, and then click the desired algorithm.

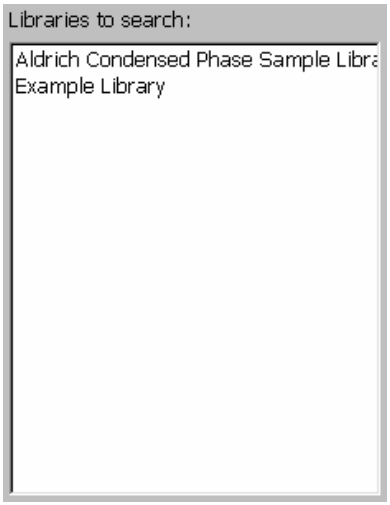
Selecting the libraries to search

The libraries that are available for searching are listed alphabetically by title in the Available Libraries box. Here is an example:





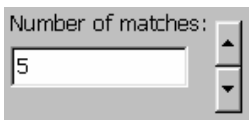
To include a library in a search, select it in the list and then click the Add button. You can include all of the listed libraries in one step by clicking the Add All button. The added libraries appear in the Libraries To Search box. Here is an example:



Note If you have a Nicolet IR200, you can select more than one library at a time: Hold down the Shift key on the keyboard and select the first and last library in a sequence to select the entire sequence, or hold down the Ctrl key and select any libraries in the list. ▲

You can remove an added library by selecting it and clicking the Remove button. (If you have a Nicolet IR200, you can remove more than one library at a time by using the techniques described in the Note above.)

Specifying the number of matches



Specify the number of library matches you would like found for the unknown spectrum by setting Number Of Matches. You can type a number in the text box or click the up and down arrow buttons to change the number. If you have a Nicolet IR100, click inside the text box to display the software keyboard. Use 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.

Setting the print options

Use the Print Options command available through the Setup button to set the options that control how spectra and reports are printed. After you set the print options, use the Print command available through the File button to print these items. See the “Printing Spectra and Reports” chapter for details. For information about reports, see “About reports” in the “Using the Software Display” chapter.

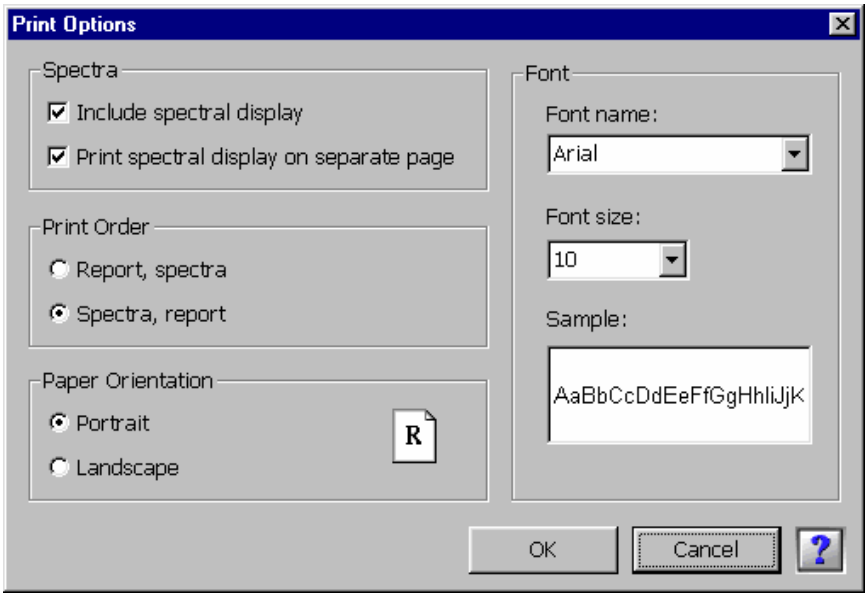
Your font name and font size settings will also be used to display information you add from the Search Results window, the Compare Results window or the Spectrum Information window to the report.

If the print option settings you need are already saved in a configuration, you can set the software in one step by opening the configuration. After you use Print Options to set the software for your preferences, you can save your settings in a configuration that can be opened later. See “Opening a configuration” and “Saving a configuration” later in this chapter for details.

Follow these steps to set the print options:

1. **Click the Setup button and then choose Print Options from the menu.**

   The print options appear:



   The appearance of this dialog box varies slightly depending on the model spectrometer you have.

2. **If you want to print spectra, turn on Include Spectral Display in the Spectra box. If you want the spectral display and report printed on separate pages, turn on Print Spectral Display On Separate Page.**

   If you choose not to print the spectra, only the report (if one exists) will be printed.

3. **If you selected Include Spectral Display in the Spectra box, use the options in the Print Order box to specify the order in which to print the spectra and the report (if one exists).**

   Select Report, Spectra to print the report first, or select Spectra, Report to print the spectra first. These options are not available if Include Spectral Display is turned off.

4. **Specify the paper orientation by selecting Portrait or Landscape in the Paper Orientation box.**

   When you make a selection, the small image of a piece of paper to the right shows how printed items will be oriented on the paper.

5. **Specify the font for printing text.**

   Use the Font Name and Font Size drop-down list boxes to select a font and a text size. Click the down arrow button to display a list of available settings, and then click the desired setting. A text example showing the selected font and size appears in the Sample box.

   Your settings will also be used to display information you add from the Search Results window, the Compare Results window or the Spectrum Information window to the report.

6. **If you have a Nicolet IR100 and want to change printers, use the Network Printer Path features as explained in the next section.**

   If you have a Nicolet IR200, you can specify a printer in the Print dialog box when you use the Print command available through the File button.

7. **When you are finished setting the print options, choose OK.**

Specifying a different printer on a Nicolet IR100

If you have a Nicolet IR100 that is connected to a network, the currently specified network printer path is shown in Network Printer Path text box in the Print Options dialog box. Follow the steps below if you want to specify a different printer for printing your spectra and reports.

Note If you want to print using only a printer connected directly to the spectrometer, no special setup is required. Skip this section. ▲

1. **Click the Setup button and then choose Print Options from the menu.**

   The print options appear.

2. **Specify the desired printer path.**

   If you know the path, you can type it in the Network Printer Path text box. The path must be a shared network resource expressed in the following general form:

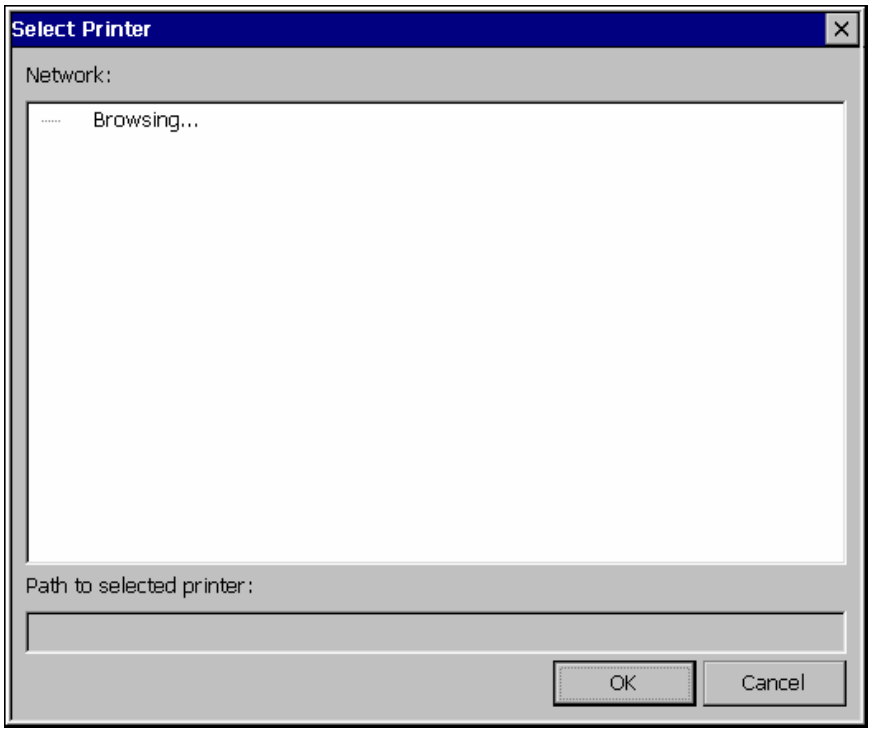
   \\computername\sharname

Note Ethernet connectors must be used to connect the computer to the network, and the computer must be properly set up in the network domain. Contact your system administrator if you need help. See "Setting up networking for a Nicolet IR100" later in this chapter for more information. ▲

   The software keyboard appears when you click inside the text box. When you are finished, go to step 3.

If you want to browse to find a printer, click the button to the right of the text box. If you know the name of the computer, you can first specify it by typing in the text box two back slashes followed by the computer name; for example, \\LAB. The Select Printer dialog box appears, and the system looks for resources on the network. (This may take a few minutes.)

Note Browsing for a printer without first entering the computer name is not available for peer-to-peer networks. ▲

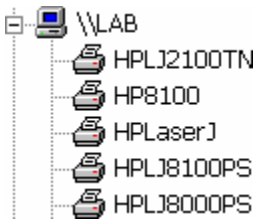


Note If your system is connected to a network, you may be prompted to enter a Windows network user name and password (these are independent of the Encompass user names and administrator password). Respond appropriately using the software keyboard that appears. Contact your system administrator if you need help. ▲

When the found drives are listed in the Network box, locate and select the desired printer. To open a drive to see the available printers, click the + sign next to the computer icon for that drive.

Note Depending on whether the drive is password-protected, you may be prompted to enter a Windows network user name and password. Respond appropriately using the software keyboard that appears. ▲

Here is an example showing the printers available through a drive that has been opened:



When you select a printer, its path appears in the Path To The Selected Printer text box. Here is an example:

3. **Choose OK.**

Opening a configuration

Use the Open Configuration command available through the Setup button to open a configuration that was previously saved. (See "Saving a configuration" later in this chapter for details.) Opening a configuration sets the software options in one step. These options include those set with the Collect Options, Display Options, Print Options and Search Options commands available through the Setup button. The use of these commands is explained earlier in this chapter.

Follow these steps to open a saved configuration:

1. **Click the Setup button and then choose Open Configuration from the menu.**

   A dialog box appears showing the available configuration files.

2. **Click the file you want to open.**

3. **Choose OK (on a Nicolet IR100) or Open (on a Nicolet IR200).**

   The software is set according to the options in the opened configuration.

   Click the button labeled "X" (on a Nicolet IR100) or choose Cancel (on a Nicolet IR200) if you want to cancel the operation.

Saving a configuration

After you have set the software options, use the Save Configuration command available through the Setup button to save your settings in a configuration that can be opened later. (See “Opening a configuration” earlier in this chapter for details.) The saved options include those set with the Collect Options, Display Options, Print Options and Search Options commands available through the Setup button. The use of these commands is explained earlier in this chapter.

Whenever you save a configuration that you consider important, we recommend making a backup copy of the file. (Save an additional copy of the file using a different filename.) This will protect you from losing the configuration in case the original file is accidentally changed or deleted.

You can delete a saved configuration by using the Delete command available through the File button. See “Deleting a file or folder” later in this chapter for details.

Follow these steps:

1. **Click the Setup button and then choose Save Configuration from the menu.**

   The Save As dialog box appears.

2. **Type a filename for the configuration in the text box.**

   If you have a Nicolet IR100, click inside the text box to display the software keyboard.

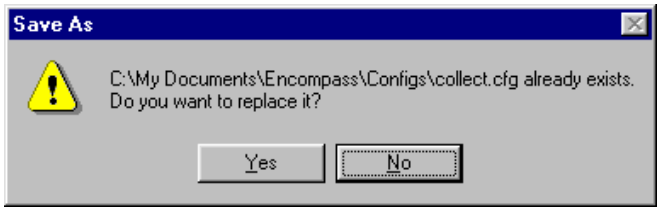
   It is not necessary to include an extension. The extension .CFG will be automatically appended to the name you type.

   Do not save the file in a directory other than the default directory (Encompass\Configs).

3. **Choose OK (on a Nicolet IR100) or Save (on a Nicolet IR200).**

   Click the button labeled “X” (on a Nicolet IR100) or choose Cancel (on a Nicolet IR200) if you want to cancel the operation.

   If you entered a filename that is already in use, a message asks you whether to replace the existing file. Here is an example:



   Choose Yes to replace the file, or choose No to return to the Save As dialog box, where you can enter a different filename.

Using System Manager

System Manager lets you control how Encompass, and thus the spectrometer, is used by other users. Typically an administrator responsible for the spectrometer sets up the system so that users must log in before using the software. The administrator can specify which configurations are available to users. If the software includes Encompass Macros, the administrator can set the system so that users have access only to macros that perform approved tasks, rather than having access to the menu buttons and commands. See the *Encompass Macros User's Guide* for complete instructions for creating and saving macros.

If you have a Nicolet IR100, you can use System Manager to connect it to a network. If you have a Nicolet IR200, your network administrator can connect its computer to a network in the same manner as any other computer running Windows.

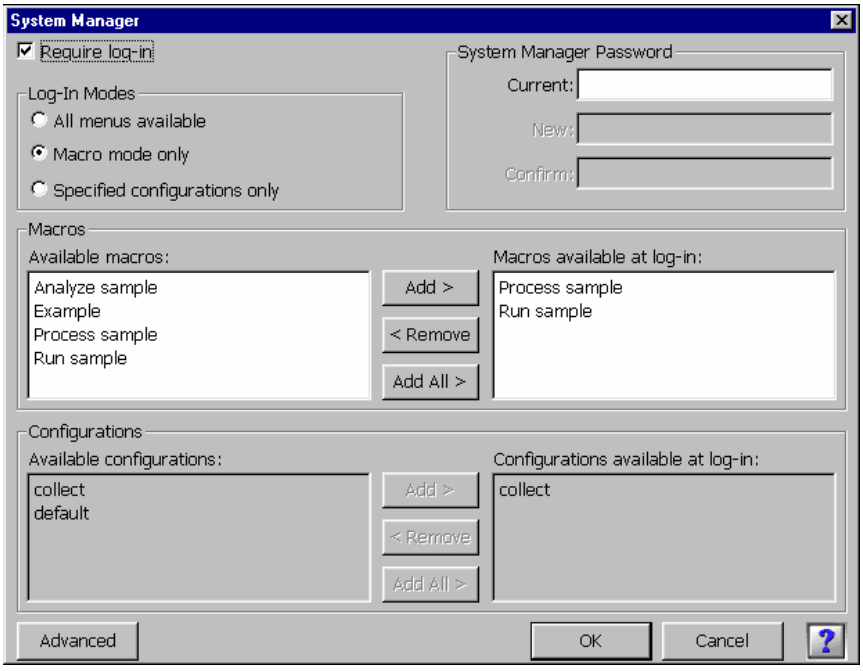
If Require Log-In is selected in System Manager, System Manager is available only if you logged in as the administrator and entered the required password.

Follow these steps to use System Manager:

1. **Click the Setup button and then choose System Manager from the menu.**

   System Manager appears showing the current system settings. Here is an example:

The appearance of this dialog box varies slightly depending on the model spectrometer you have.



   The availability of features in System Manager changes when you change the settings.

2. **If you want to require users to log in before using Encompass, turn on Require Log-In and then select a mode in the Log-In Modes box.**

   Logging in involves entering a user name and may require selecting a configuration or macro when the software starts. If you don't require that users log in, all features of the software will be available to everyone. If you turn off Require Log-In, go to step 4.

   If you turn on Require Log-In, you can specify a different system manager password (explained in the next step) and must select one of three modes in the Log-In Modes box. These modes offer different levels of control over which features will be available to users:

   - The **All Menus Available** setting gives users access to all the features of the software except System Manager and these buttons in the Library Organizer: Info (for libraries), Compress and Delete (for libraries and library spectra).

   - If you purchased Encompass Macros and want to require users to perform operations only with specified macros, select **Macro Mode Only** and then specify the macros. The menu buttons and commands will not be available to users if you select this mode.

     The Available Macros box lists the macros that have been created and saved. To make some of these available to users, select them and then click the Add button to add them to the list of macros in the Macros Available At Log-In box. You can click the Add All button to add all of the saved macros to the list. To remove a macro from the Macros Available At Log-In box, select it and then click the Remove button.

- If you want to require users to use only specified configurations, select **Specified Configurations Only** and then specify the configurations. The configurations contain option settings that affect collecting and displaying spectra, printing, and searching spectral libraries. Users will not be able to change the settings within a configuration. All software features will be available except those accessed through the Setup button, and the Library Organizer command accessed through the Analyze button.

  The Available Configurations box lists the configurations that have been saved. To make some of these available to users, select them and then click the Add button to add them to the list of configurations in the Configurations Available At Log-In box. You can click the Add All button to add all of the saved configurations to the list. To remove a configuration from the Configurations Available At Log-In box, select it and then click the Remove button.

Regardless of which operation mode you select, the system administrator can always have access to every software feature, including System Manager, by simply entering the system manager password when logging in.

3. Change the administrator's password if desired.

To do this, type the current password in the Current text box, type a new password in the New text box, and then type the new password in the Confirm text box. If you have a Nicolet IR100, click inside the text box to display the software keyboard. If you forget or lose the administrator's password, contact Technical Support at one of the numbers given in the "Questions and concerns" section in the "Welcome" chapter for assistance.

Note When you first use the software, no administrator password exists. To establish an initial password, type a space in the Current text box to make the New and Confirmed text boxes available, and then type the desired password in the New and Confirm text boxes, as described above. ▲

If you accidentally type an incorrect password, the software informs you and allows you to reenter the password.

4. **If you have a Nicolet IR100 and want to set up its network connection, use the Advanced button as explained in the next section.**

   The Advanced button is available only if you have a Nicolet IR100.

5. **When you are finished using System Manager, choose OK.**

   Choose Cancel if you want to cancel your changes. (Changes you made with the Advanced button are not canceled.)

Setting up networking for a Nicolet IR100

If you have a Nicolet IR100 and want to connect it to a network, use the Advanced button in System Manager to set the options that establish the connection. (If you have a Nicolet IR200, your network administrator can connect its computer to a network in the same manner as any other computer running Windows.)

Note Depending on the amount of traffic handled by your network, the screen of the Nicolet IR100 may sometimes flicker. This is caused by the network sending the Nicolet IR100 data packets from various network computers not needed for its operation. You can solve this problem by installing a network switch hub, an intelligent device that reads incoming data packets and then routes them appropriately. Over time it learns how your network functions and stops sending the unneeded data to the spectrometer. ▲

It is possible to connect the Nicolet IR100 to a wireless network. This requires that a wireless network bridge be connected to the Ethernet port of the spectrometer. The type of network bridge must be compatible with the wireless network already set up. You can connect the spectrometer to an existing network in infrastructure mode or to another computer in a peer-to-peer, ad-hoc mode. Both network types require a wireless access point in the network. Select a network bridge that can be set up through a network browser. Set up the network bridge on another computer, and then connect it to the Nicolet IR100. Set the network settings by using the Advanced button in System Manager. Follow the instructions provided by the manufacturer of the network bridge, or consult your network administrator to set up the network correctly.

The following sections explain how to...

- Set up conventional Windows networking.
- Set up peer-to-peer networking.
- Specify a network path for opening and saving spectra or reports.

Setting up conventional Windows networking

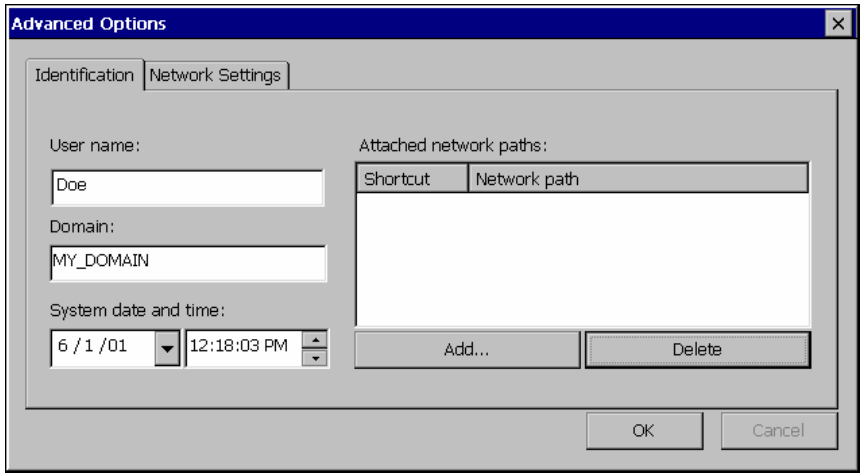
Follow the steps below to set up conventional Windows networking for your Nicolet IR100. Typically this type of networking is used for networks that include multiple domains and one or more servers. Since setting up networking requires specialized knowledge, we recommend that it be performed by your network administrator.

1. **Click the Setup button and then choose System Manager from the menu.**

   System Manager appears.

2. **Click the Advanced button.**

   The Advanced Options dialog box appears. Here is an example:



3. **Type your user name in the User Name text box on the Identification tab.**

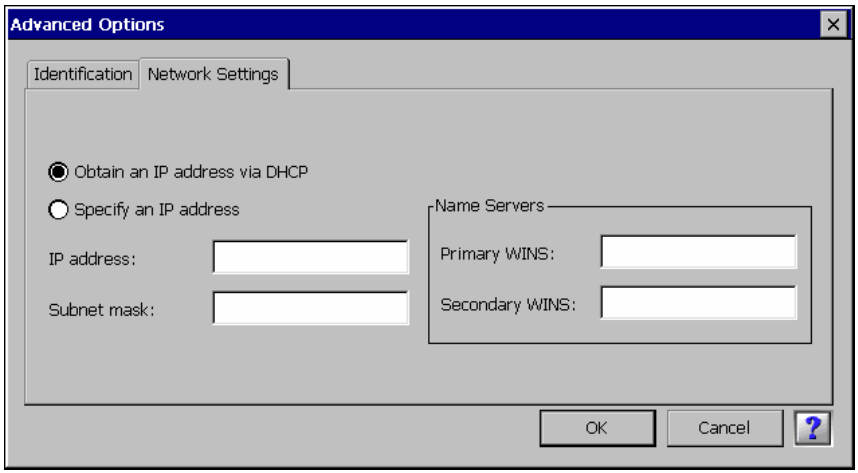
   The name must be one that can be recognized by the network.

4. **Type the name of the network domain to which you want to connect in the Domain text box.**

5. **Use the System Date And Time features to specify the current date and time.**

6. **On the Network Settings tab select an IP address option.**

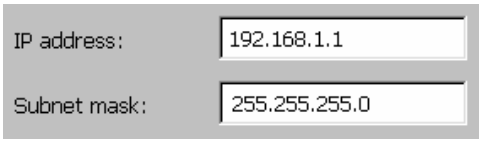
Here is an example showing the Network Settings tab:



Each system connected to the network needs a unique numerical IP (Internet Protocol) address.

- If the network has a DHCP server and you want it to assign the IP address automatically, select Obtain An IP Address Via DHCP. When you connect to the network, it will assign your system an IP address that is used only for the duration of that connection.

- If you want to specify a fixed IP address, select Specify An IP Address. Then type the address in the IP Address text box and the subnet mask in the Subnet Mask text box. The subnet mask tells the network how much of the IP address is controlled by the network router. Here is an example:



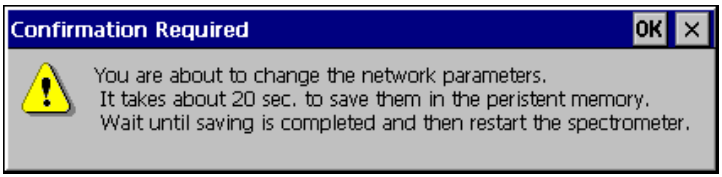
The IP address setting and other settings on this tab will be saved in the system registry.

7. **Type the addresses of the primary and secondary WINS name servers in the Primary WINS and Secondary WINS text boxes, respectively.**

   The name servers determine the numerical addresses of the spectrometer in the domain that you entered on the Identification tab.

8. **Choose OK.**

   A message appears:



9. **Choose OK.**

10. **Wait at least 20 seconds and then turn off the spectrometer power and turn it back on.**

    The power switch is on the rear panel of the spectrometer.

    This puts your network settings into effect and establishes your network connection. If you want to specify a path on the network for opening and saving spectra or reports, use the procedure in "Specifying a network path for opening and saving spectra and reports."

Setting up peer-to-peer networking

Follow the steps below to set up peer-to-peer networking for your Nicolet IR100. This type of networking is used for connecting two or more computers in a network that does not include a server. You can use peer-to-peer networking to connect the built-in computer of your Nicolet IR100 to one or more workstation computers running Windows. You can then access a shared network folder or printer from your Nicolet IR100.

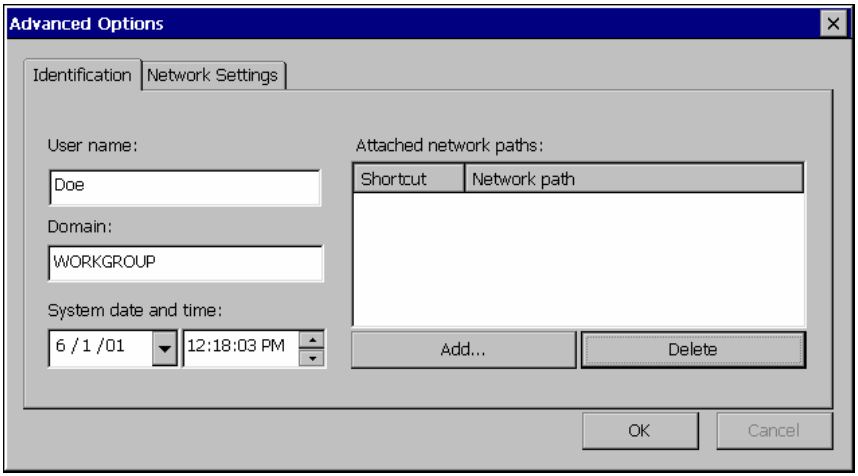
Note The following procedure gives a typical example of how to set up peer-to-peer networking for a Nicolet IR100. The specific Windows features used may vary depending on the version of Windows installed on your workstation computers. If the computers are connected to an administrated institutional network, ask a network administrator for assistance. In this procedure we will assume that the computers, as well as the folder or printer you want to share, have already been set up using Windows administrative features. ▲

1. **Click the Setup button and then choose System Manager from the menu.**

   System Manager appears.

2. **Click the Advanced button.**

   The Advanced Options dialog box appears. Here is an example:



3. **Type your user name in the User Name text box on the Identification tab.**

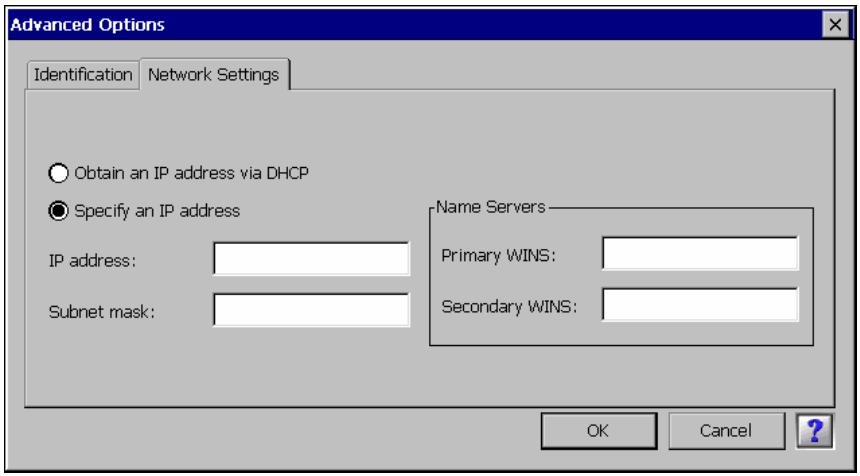
   If you want to use a shared folder on another computer in the network and the folder does not have password protection, you can use any name. If the shared folder has password protection, use a name that is recognized by that computer.

4. **Type the name of your workgroup in the Domain text box.**

   The name must match the workgroup name used by the other computers on the network. See the preceding illustration for an example.

5. **Use the System Date And Time features to specify the current date and time if they are not already specified.**

6. **On the Network Settings tab select the Specify An IP Address option.**



7. **Type an available IP address in the IP Address text box.**

   Each system connected to the network needs a unique numerical IP (Internet Protocol) address. Here is an example:

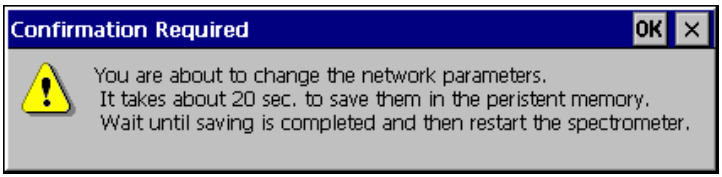
   The IP address setting and other settings on this tab will be saved in the system registry. If your computers are connected to an administrated institutional network, ask a network administrator for the IP address.

8. **In the Subnet Mask text box, type a subnet mask that matches the subnet mask specified on the other computers.**

   The subnet mask tells the network how much of the IP address is controlled by the network router. One option is to use 255.255.255.0 for all of the systems on the network.

9. **Choose OK.**

   A message appears:



10. **Choose OK.**

11. **Wait at least 20 seconds and then turn off the spectrometer power and turn it back on.**

    The power switch is on the rear panel of the spectrometer.

    This puts your network settings into effect and establishes your network connection.

    If you want to specify a path on the network for opening and saving spectra or reports, use the procedure in “Specifying a network path for opening and saving spectra and reports.”

Tip Make sure the networking settings on the desktop computers on the network are correct. This includes the Client For Microsoft Network and File And Printer Sharing features (or equivalent features in your version of Windows).

Set the TCP/IP parameters to match the address range used by the Nicolet IR100. For example, the IP address 192.168.1.2 could be used with the address shown in step 7. The specified IP addresses of the computers must be consistent for networking to work properly.

Make sure the workgroup name matches the name you entered in step 4.

If you change any settings, restart the computer. ▲

Specifying a network path for opening and saving spectra or reports

If you have a Nicolet IR100 that is connected to a network, you can use the Advanced button to specify a network path for opening and saving spectra and reports. We recommend that this procedure be performed with the help of the system administrator.

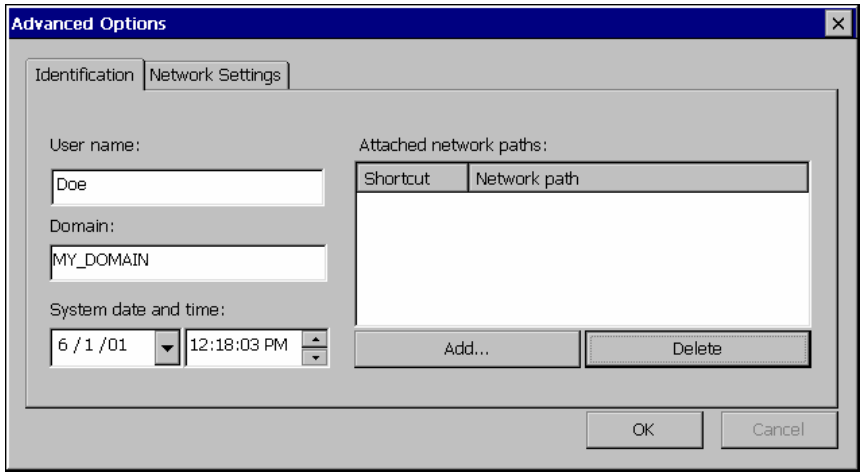
Follow these steps:

1. **Click the Setup button and then choose System Manager from the menu.**

   System Manager appears.

2. **Click the Advanced button.**

The Advanced Options dialog box appears. Here is an example:



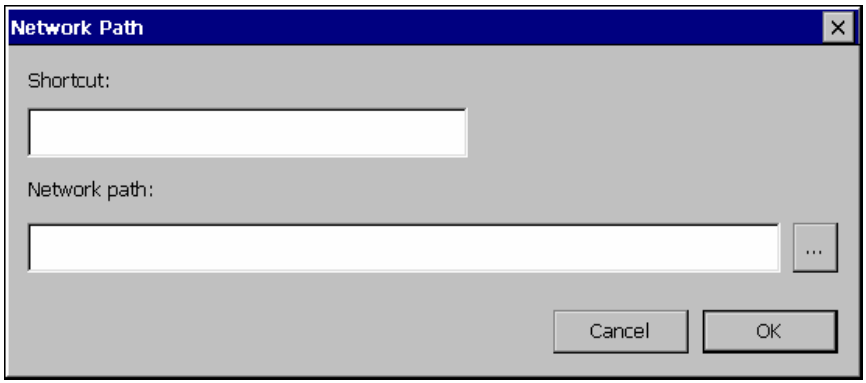
The network paths that are currently available for opening and saving spectra and reports are listed in the Attached Network Paths box on the Identification tab. For each path the Shortcut column shows the path's shortcut name, and the Network Path column shows the full pathname. Shortcuts are used as a convenient way to refer to paths.

You can delete a listed path by clicking it and then choosing Delete.

3. **If you want to add a network path, choose Add.**

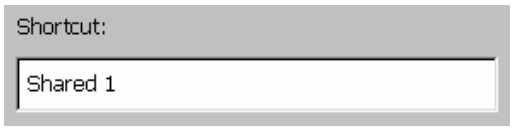
Note You may be prompted to enter a Windows network user name and password (these are independent of the Encompass user names and administrator password). Respond appropriately using the software keyboard. The name and password you enter must be recognized in the domain specified on the Identification tab. Contact your system administrator if you need help. ▲

The Network Path dialog box appears:



4. **Enter a shortcut name for the path in the Shortcut text box.**

   Here is an example:



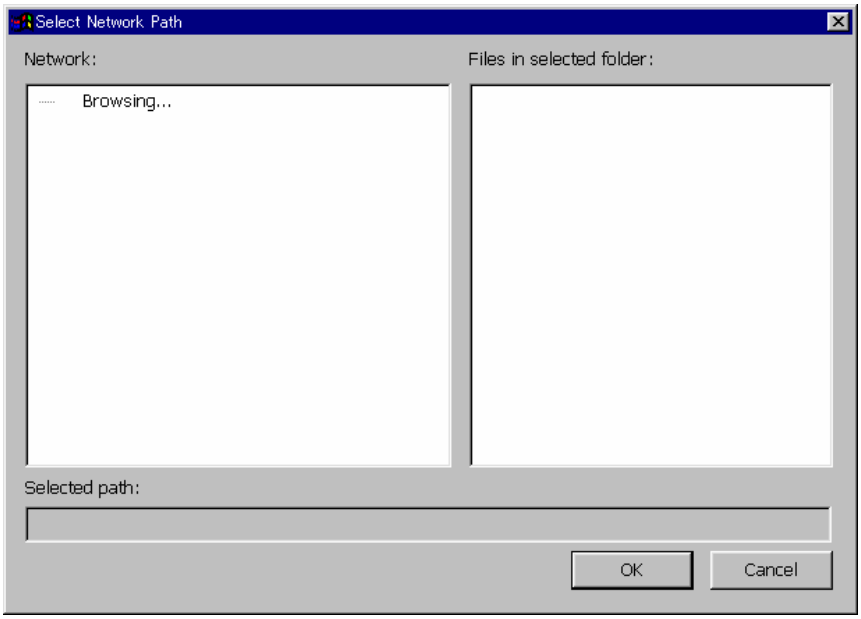
   The shortcut name will be used to name a folder within the Network folder. You will be able to locate and use this folder when you later open or save a spectrum or report.

5. **Specify the pathname of the network path.**

   If you know the pathname, you can type it in the Network Path text box. Here is an example:

If you don't know the full pathname, you can browse for the desired path by clicking the button to the right of the text box. If you know the name of the computer, you can first specify it by typing in the text box two back slashes followed by the computer name; for example, \\LAB. When you click the button, the Select Network Path dialog box appears, and the system looks for paths on the network. (This may take a few minutes.)

Note Browsing for a path without first entering the computer name is not available for peer-to-peer networks. ▲



When the found paths are listed in the Network box, locate and select the desired folder. To open a drive to see the available folders, click the + sign next to the computer icon for that drive. Here is an example showing a folder that is available through a drive that has been opened:

When you select a folder, any files it contains are listed in the Files In Selected Folder box.

When you are finished, choose OK. The path appears in the Network Path text box.

6. **Choose OK.**

   The new path appears in the Attached Network Paths box.

   You can add another path by repeating steps 3 through 6.

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

Note You may be prompted to enter a Windows user name and password (these are independent of the Encompass user names and administrator password). Respond appropriately using the software keyboard. Contact your system administrator if you need help. ▲

8. **Choose OK to close System Manager.**

Using macros

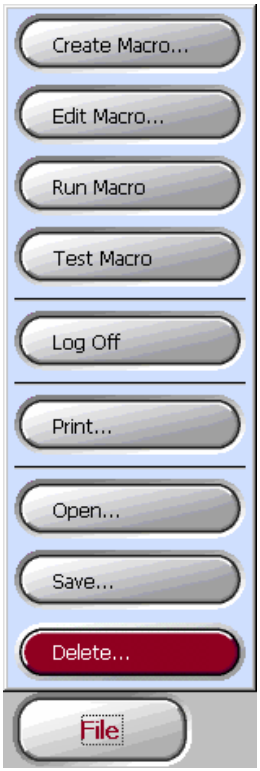
If you purchased Encompass Macros, you can create and use macros to perform many tasks with Encompass. A macro is a sequence of software operations that, once started, run in the specified order until completion. There are two important advantages to using a macro: You can perform several operations by initiating just one macro—and once the macro is set up and saved, you can run it whenever you need to.

See the *Encompass Macros User's Guide* for complete information on creating and using macros.

Macro mode

If Macro Mode Only is selected in System Manager, users other than the system administrator do not have access to the menu buttons when they log into Encompass. Instead, they can only run macros that have been specified in System Manager. See "Using System Manager" earlier in this chapter for information on turning Macro Mode Only on or off and specifying macros. See "Starting the software" in the "Getting Started" chapter for information on logging into Encompass and selecting macros to run in macro mode.

Deleting a file or folder



Use the Delete command available through the File button to delete a file containing a spectrum, report, macro or configuration, or an empty folder (on a Nicolet IR100 only). Follow these steps:

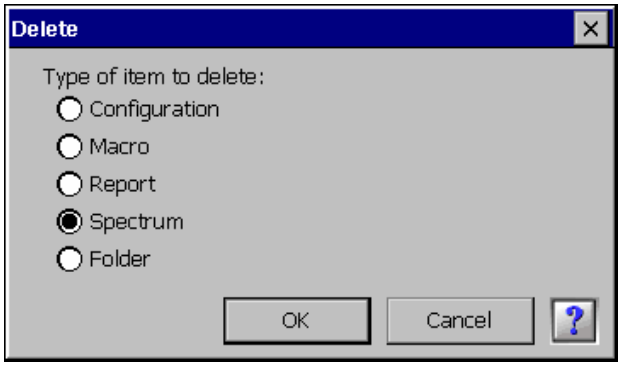
1. **If you have a Nicolet IR100 and want to delete a file or empty folder from an optional flash memory card, insert the card into the flash memory card slot on the front of the spectrometer.**

   Flash memory cards are sensitive to static electricity. When handling them, always follow the precautions given in "Using flash memory cards" later in this chapter.

   See "Using flash memory cards" later in this chapter for an illustration showing how to insert the card.

2. **Click the File button and then choose Delete from the menu.**

   The Delete dialog box appears:



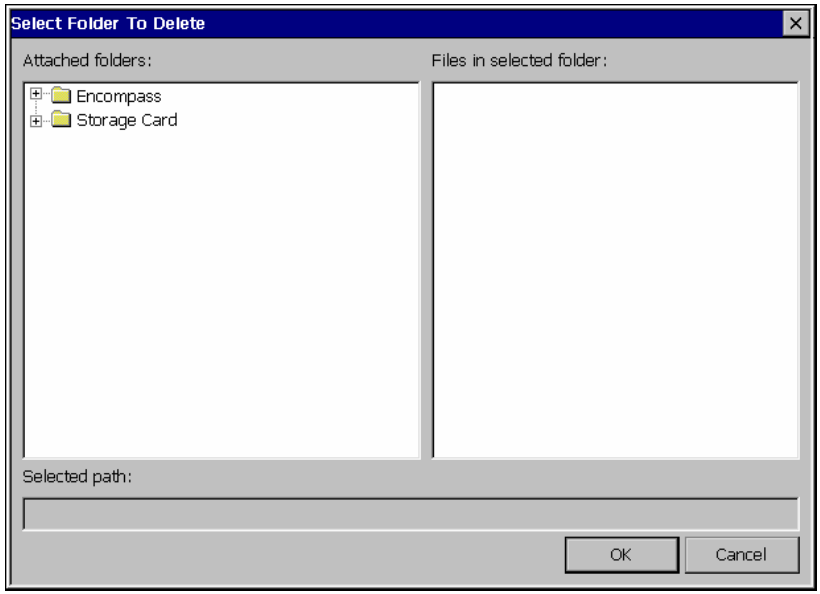
Note The Folder option appears only if you have a Nicolet IR100. If you have a Nicolet IR200, you can delete folders by using Windows Explorer or My Computer. See your Windows documentation if you need help. ▲

3. **Select the type of item you want to delete.**

4. **Choose OK.**

   - If you selected any type other than Folder, a dialog box appears showing the available files of the type you specified. Go to step 7.

   - If you selected Folder, the Select Folder To Delete dialog box appears. Here is an example:



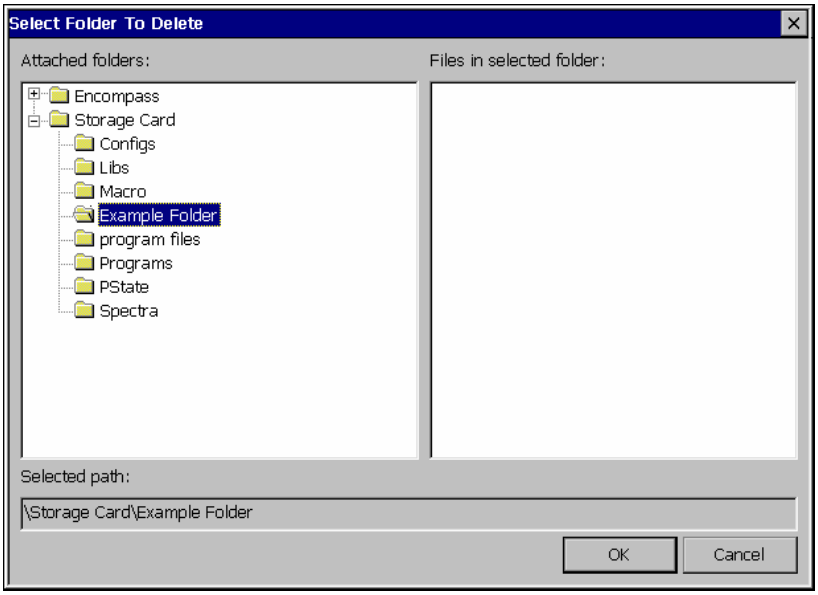
   Go to the next step.

5. **In the Attached Folders box, locate and select the empty folder you want to delete.**

   To view the folders contained in a folder, click the + sign to the left of the folder icon.

   To select a folder for deletion, click it. Here is an example:

Only empty folders can be deleted.



   If the selected folder contains files, they are listed in the Files In Selected Folder box. A folder containing files cannot be deleted.

6. **Choose OK.**

   The procedure is finished.

7. **If you are deleting a file stored on a flash memory card, display the contents of the card.**

   To do this, click the  button until “My Computer” appears near the top of the dialog box. Then double-click the folder named “Storage Card.”

8. **Click the file you want to delete.**

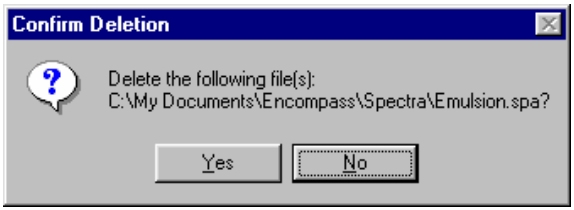
   You can change directories or drives to locate a file.

   If you have a Nicolet IR200, you can delete more than one file at a time: Hold down the Ctrl key and click each file you want to delete, or hold down the Shift key and click the first and last files in a sequence of files.

9. **Choose OK (on a Nicolet IR100) or Delete (on a Nicolet IR200).**

   Click the Esc key or the button labeled “X” (on a Nicolet IR100) or choose Cancel (on a Nicolet IR200) if you want to cancel the operation.

   A message asks whether to delete the file (or files). Here is an example:



10. **Choose Yes.**

    Choose No if you want to cancel the operation.

Using flash memory cards

If you have a Nicolet IR100, you can store spectra, reports, spectral libraries and macros on CompactFlash™ flash memory cards. (See "Saving a spectrum or report" in the "Opening and Saving Spectra and Reports" chapter and "Copying a library to a new location" in the "Analyzing Spectra" chapter of this manual and "Backing up a macro" in the "Editing a Macro" chapter of the *Encompass Macros User's Guide*.) You can also buy and use spectral libraries that come on a flash memory card (see the next section).

Since the cards are sensitive to static electricity, it is important that you handle and store the cards properly to protect the files they contain. Read and follow the precautions below.

Important Failure to follow these precautions may result in damage to your flash memory cards and loss of data. ▲

- When you receive a flash memory card, it is in a special protective case. Leave the card in the case until you are ready to use it. Once you remove the card from the case, do not set it down until you have installed it in the flash memory card slot on the front of the spectrometer (see the following illustration).

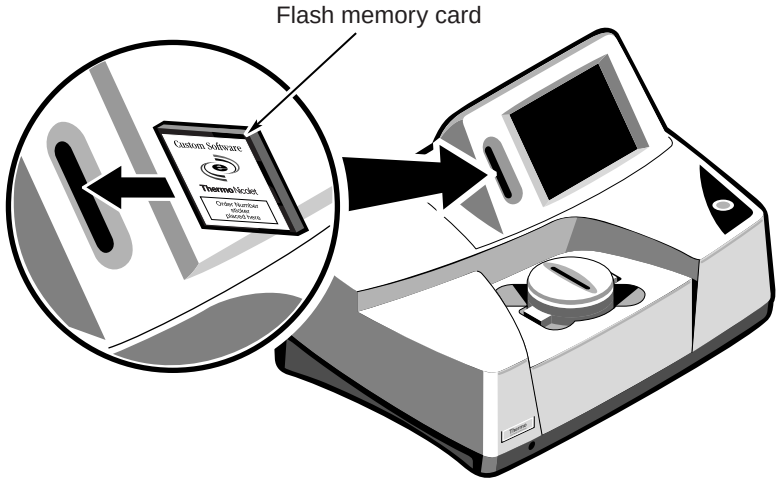
- Before handling a flash memory card, equalize the static electricity between the card and the spectrometer by touching the rear panel of the spectrometer with one hand and the card with your other hand. Do not set the card down until it is installed in the flash memory card slot on the front of the spectrometer (see the following illustration).

- When you are not using a flash memory card, store it in its protective case.

- Do not store flash memory cards near strong electrostatic, electromagnetic, magnetic or radioactive fields. Keep your cards dry and away from harsh chemicals and extreme temperatures.

- If you need to transport a flash memory card, always place it in its protective case or in an antistatic bag or container.

To use a flash memory card, insert it into the slot on the front of the spectrometer as shown below.



Note When you insert a flash memory card that contains a new version of Encompass software, a message asks you whether to update the software on your system. Respond appropriately. For more information see the installation instructions that came with the software. ▲

When you are finished using the card, press the black button below the card and pull the card out of the slot.

Viewing a list of the libraries contained on a flash memory card

If you buy additional spectral libraries from us for your Nicolet IR100, they are shipped on a flash memory card. You can see a list of the libraries contained on the card by following these steps:

1. **Insert the card into the slot on the front of the spectrometer.**

2. **Click the File button and choose Open.**

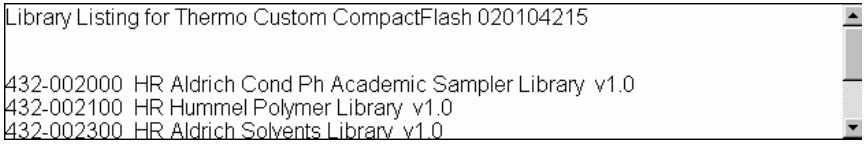
3. **In the dialog box that appears, set Type to Report and choose OK.**

4. **Display the contents of the card.**

   To do this, click the  button until "My Computer" appears near the top of the dialog box. Then double-click the folder named "Storage Card."

5. **Click the file named LIBLIST.TXT and choose OK.**

   The list of libraries appears in the report. (If the report is not displayed, use Show Report available through the View button to display it.) Here is an example:



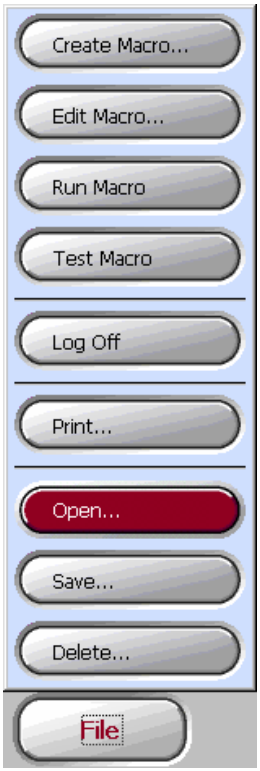
   The text above the list shows the serial number of the flash card. In the list, the part number of each library is shown, followed by the library title.

Opening and Saving Spectra and Reports

You can use commands available through the File button to open previously saved spectra and reports and to save collected spectra and reports you have generated. The next sections explain how to perform these tasks.

Note If your Nicolet IR100 is connected to a network, you can specify a path for opening and saving spectra or reports. See “Specifying a network path for opening and saving spectra or reports” in the “Software Management” chapter for details. ▲

Opening a spectrum or report



Use the Open command available through the File button to open a spectrum or report that was previously saved. Follow these steps:

1. **If you have a Nicolet IR100 and want to open a file that was saved on an optional flash memory card, insert the card into the flash memory card slot on the front of the spectrometer.**

   Flash memory cards are sensitive to static electricity. When handling them, always follow the precautions given in "Using flash memory cards" in the "Software Management" chapter. Also see that section for an illustration showing how to insert the card.

2. **Click the File button and then choose Open from the menu.**

   The Open dialog box appears showing the available spectral data files. (You can display the available report files in the next step.)

3. **If you want open a spectrum, set Type (on a Nicolet IR100) or Files Of Type (on a Nicolet IR200) to Spectrum. If you want to open a report, set the option to Report.**

4. **If you are opening a file stored on a flash memory card, display the contents of the card.**

   To do this, click the  button until "My Computer" appears near the top of the dialog box. Then double-click the folder named "Storage Card."

5. **Click the file you want to open.**

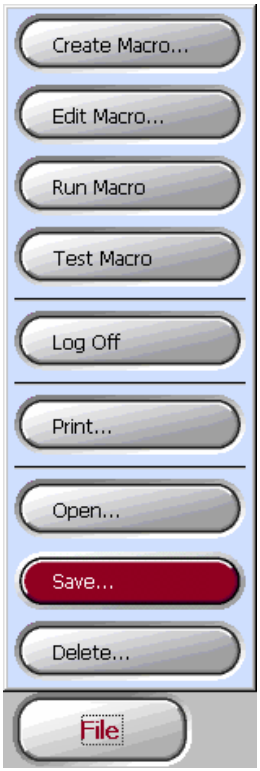
   You can change directories or drives to locate a file.

6. **Choose OK (on a Nicolet IR100) or Open (on a Nicolet IR200).**

   Click the button labeled “X” (on a Nicolet IR100) or choose Cancel (on a Nicolet IR200) if you want to cancel the operation.

   If you opened a spectrum, it appears in the spectral display. If you opened a report, its contents are added to the current report, at the end. (If the report is not displayed, use Show Report available through the View button to display it. See “Displaying or hiding the report” in the “Using the Software Display” chapter earlier in this manual for details.)

Saving a spectrum or report



Use the Save command available through the File button to save the selected spectrum or the current report. Reports are saved in plain text format.

If you have a Nicolet IR100, you can save these items in the system's internal flash memory, on an optional external flash memory card, or in a network location. If you have a Nicolet IR200, you can save spectra and reports on the computer's hard disk, on other disks you provide, or in a network location.

If you have a Nicolet IR100, save spectra and reports only in directories within the Encompass, Storage Card or Network directories (if present). Files saved in other directories will be lost when you turn off the spectrometer power. The default directory (Spectra) for saving spectra and reports is within the Encompass directory. See "Specifying a network path for opening and saving spectra or reports" later in this chapter for more information on saving spectra and reports on a network.

You cannot save a spectrum exported from a commercial library. See "Exporting a library spectrum" in the "Analyze" chapter for information on exporting library spectra.

Whenever you save a spectrum or report that you consider important, we recommend making a backup copy of the file. (Save an additional copy of the file using a different filename.) This will protect you from losing data in case the original file is accidentally changed or deleted.

If you want to save any results that you have added to a report, be sure to save the report before exiting Encompass. The report display will be cleared when you exit.

You can set the software to save spectra automatically after collection. See "Saving collected spectra automatically" in the "Software Management" chapter for details.

You can delete a saved spectrum or report by using the Delete command available through the File button. See “Deleting a file or folder” in the “Software Management” chapter for details.

Note Since reports are saved as text files (having the extension .TXT), you can open and edit a saved report using Notepad, WordPad, Microsoft Word or other programs that open text files. Since a text file does not contain formatting information, a report you open in another program may look different from the way it looked in the Encompass window. ▲

Follow these steps to save the selected spectrum or a report:

1. **If you have a Nicolet IR100 and want to save the spectrum or report on a flash memory card, insert the card into the flash memory card slot on the front of the spectrometer.**

Important Flash memory cards are sensitive to static electricity. When handling them, always follow the precautions given in “Using flash memory cards” in the “Software Management” chapter. ▲

See “Using flash memory cards” in the “Software Management” chapter for an illustration showing how to insert the card.

2. **Click the File button and then choose Save from the menu.**

The Save As dialog box appears.

3. **If you are saving a spectrum, set Type (on a Nicolet IR100) or Save As Type (on a Nicolet IR200) to Spectrum. If you are saving a report, set the option to Report.**

4. **If you have a Nicolet IR200, you can change directories to save the file in a different directory. If you have a Nicolet IR100 and are saving a file on a flash memory card or in a network location, display the contents of the card or the network location as explained below.**

   To display the contents of the card, click the  button until "My Computer" appears near the top of the dialog box. Then double-click the folder named "Storage Card."

   To display the network location, click the  button until "Network" appears near the top of the dialog box. Then double-click the folder in which you want to save the file.

5. **Type a filename for the spectrum or report in the text box.**

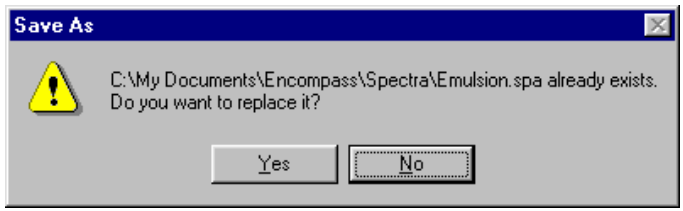
   If you have a Nicolet IR100, click inside the text box to display the software keyboard.

   It is not necessary to include an extension. The correct extension (.SPA for a spectrum, or .TXT for a report) will be automatically appended to the name you type.

6. **Choose OK (on a Nicolet IR100) or Save (on a Nicolet IR200).**

   Click the button labeled "X" (on a Nicolet IR100) or choose Cancel (on a Nicolet IR200) if you want to cancel the operation.

If you entered a filename that is already in use, a message asks you whether to replace the existing file. Here is an example:

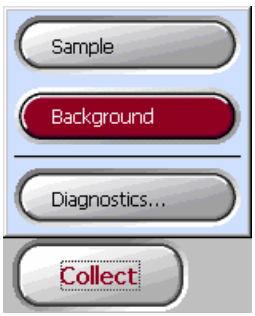


Choose Yes to replace the file, or choose No to return to the Save As dialog box, where you can enter a different filename.

Collecting Spectra

You can use Encompass with your spectrometer to collect background spectra and spectra of your sample materials. The next sections explain in detail how to use the Background and Sample commands to collect these spectra.

Collecting a background



Use the Background command available through the Collect button to collect a background spectrum. A background measures the response of the spectrometer without a sample in place. “Ratioing” a sample spectrum against a background eliminates signals that are due the characteristics of the spectrometer components, as well as absorptions caused by water vapor and carbon dioxide.

Follow these steps to collect a background:

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

   If you are using the Transmission accessory, pull the sample out of the slot in the accessory. If you are using a different accessory, remove any sample material as explained in the manual that came with the accessory.

   If you have a lithium tantalate detector, wait 10 seconds for the detector to stabilize before starting data collection (in step 3).

2. **Use the Collect Options command available through the Setup button to set the data collection options.**

Note If you have just installed your system and are collecting your first spectra, the default data collection option settings should work well. You can skip this step. ▲

The options let you specify the resolution, number of scans, and other items. See “Setting the data collection options” in the “Software Management” chapter for details.

If the desired option settings have been saved in a configuration, simply open that configuration. See “Opening a configuration” in the “Software Management” chapter for more information.

You can skip this step if you know the options are already set correctly.

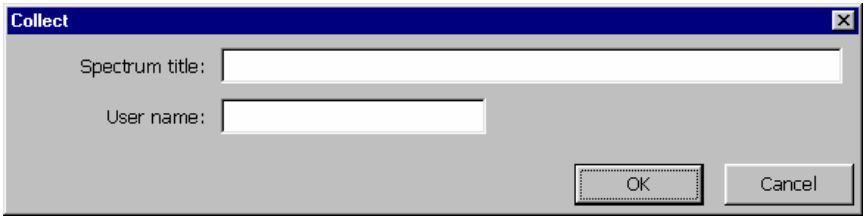
Note If you have a Nicolet IR100 and plan to save collected spectra automatically on a flash memory card, make sure the card is installed in the flash memory card slot on the front of the spectrometer. Flash memory cards are sensitive to static electricity. When handling them, always follow the precautions given in “Using flash memory cards” in the “Software Management” chapter. See “Saving collected spectra automatically” in that chapter for more information about saving spectra automatically. ▲

3. **Click the Collect button and then choose Background from the menu.**

4. **If you are prompted to enter a spectrum title or your name, enter the appropriate information and then choose OK.**

   The settings of the data collection options determine whether and how you are prompted. See “Prompting for a user name” and “Prompting for a spectrum title” in the “Software Management” chapter for more information.

Here is an example of a prompt:



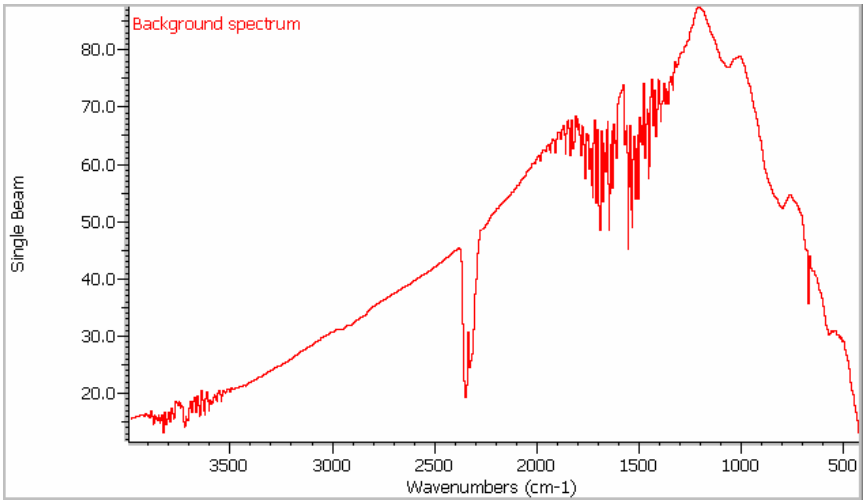
If you have a Nicolet IR100, click inside the text box to display the software keyboard.

Choose Cancel if you want to end the procedure.

If you choose OK, or if you are not prompted for a title or name, a gauge shows the progress of the collection. The number of scans collected so far and the total number of scans appear above the gauge.

You can cancel the collection at any time by choosing Cancel.

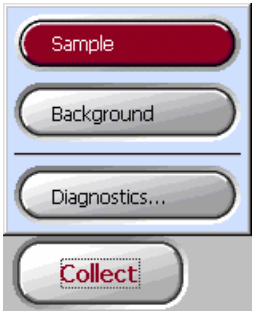
When the collection is finished, the background appears in the spectral display if Show Background After Collection is selected in the data collection options. (See “Displaying the background after it is collected” in the “Software Management” chapter for more information.)



Regardless of whether the background is displayed, it is placed in memory so that it can be used to ratio sample spectra.

If the background was not saved automatically, but it is displayed and you want to save it, use the Save command available through the File button. See “Saving collected spectra automatically” in the “Software Management” chapter and “Saving a spectrum or report” in the “Opening and Saving Spectra and Reports” chapter for more information.

Collecting a sample spectrum



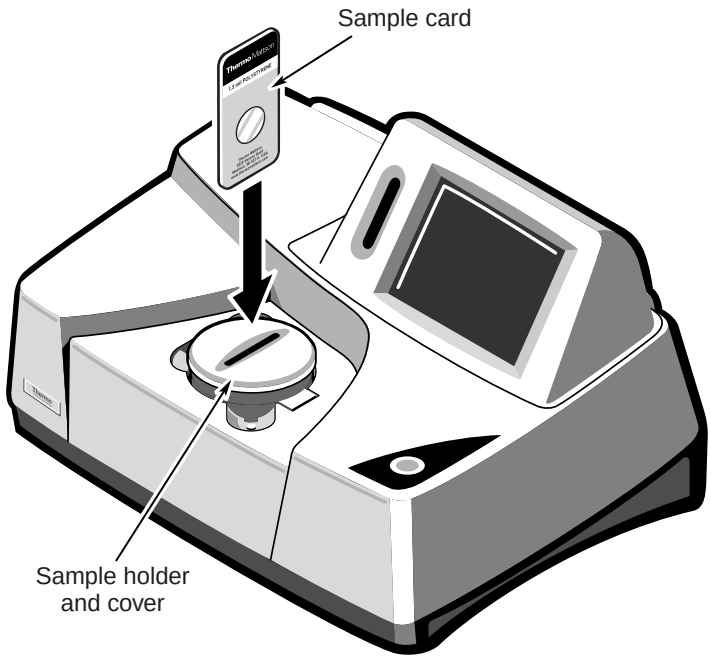
Use the Sample command available through the Collect button to collect a spectrum of a sample. Before it is displayed, the collected spectrum is automatically ratioed against the current background to produce a spectrum with the specified Y-axis format, either absorbance or % transmittance. See “Displaying spectra in absorbance or % transmittance” in the “Software Management” chapter for more information.

If Data Format in the data collection options is set to Interferogram, the data is not ratioed and appears in the spectral display as an interferogram. See “Specifying the format of the collected data” in the “Software Management” chapter for details.

Follow these steps to collect a sample spectrum:

1. **Install the sample.**

   If you are using the Transmission accessory, slide the sample into the slot in the accessory as shown below. If you are learning how to collect your first sample spectrum, you can use the provided polystyrene sample card.



   If you are using a different accessory, see the manual that came with it for instructions.

   If you have a lithium tantalate detector, wait 10 seconds for the detector to stabilize before starting data collection (in step 3).

2. **Use the Collect Options command available through the Setup button to set the data collection options.**

Note If you have just installed your system and are collecting your first spectra, the default data collection option settings should work well. You can skip this step. ▲

The options let you specify the resolution, number of scans, and other items. See “Setting the data collection options” in the “Software Management” chapter for details.

If the desired option settings have been saved in a configuration, simply open that configuration. See “Opening a configuration” in the “Software Management” chapter for more information.

You can skip this step if you know the options are already set correctly.

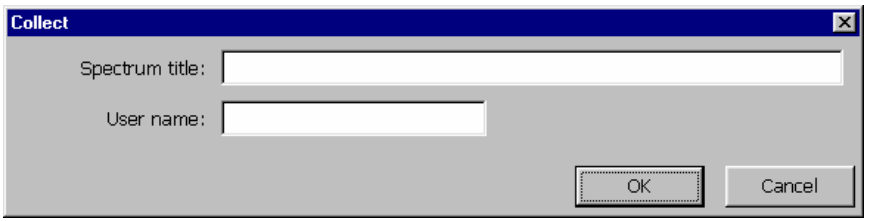
Note If you have a Nicolet IR100 and plan to save collected spectra automatically on a flash memory card, make sure the card is installed in the flash memory card slot on the front of the spectrometer. Flash memory cards are sensitive to static electricity. When handling them, always follow the precautions given in “Using flash memory cards” in the “Software Management” chapter. See “Saving collected spectra automatically” in that chapter for more information about saving spectra automatically. ▲

3. **Click the Collect button, choose Sample from the menu and then follow any instructions that appear.**

If a prompt says that there is no background, choose OK and then collect a background (without a sample installed) before collecting the sample spectrum. See “Collecting a background” earlier in this chapter for details.

If a prompt says that the background resolution does not match the current resolution (set in the data collection options), choose OK and then collect a background (without a sample installed) with the correct resolution before collecting the sample spectrum. See “Setting the resolution” in the “Software Management” chapter for more information.

If you are prompted to enter a spectrum title or your name, enter the appropriate information and then choose OK. The settings of the data collection options determine whether and how you are prompted. See “Prompting for a user name” and “Prompting for a spectrum title” in the “Software Management” chapter for more information. Here is an example of a prompt:



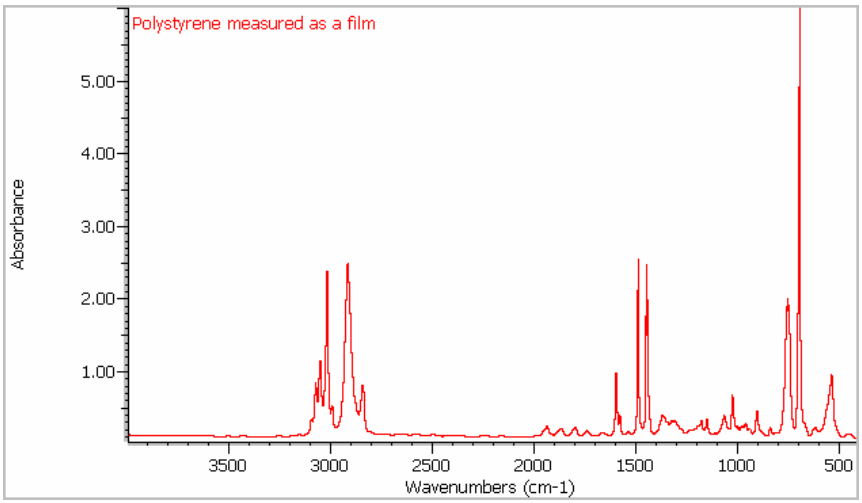
If you have a Nicolet IR100, click inside the text box to display the software keyboard.

Choose Cancel if you want to end the procedure.

If you choose OK, or if you are not prompted for a title or name, a gauge shows the progress of the collection. The number of scans collected so far and the total number of scans appear above the gauge.

You can cancel the collection at any time by choosing Cancel.

When the collection is finished, the sample spectrum appears in the spectral display.



If the spectrum was not saved automatically but you want to save it, use the Save command available through the File button. See "Saving collected spectra automatically" in the "Software Management" chapter and "Saving a spectrum or report" in the "Opening and Saving Spectra and Reports" chapter for details.

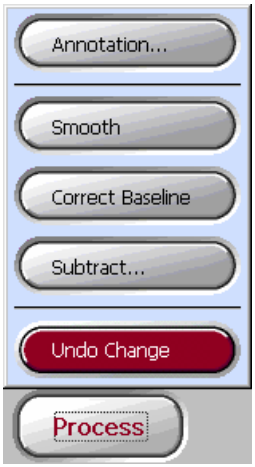
Note If you have just collected your first sample spectrum and want to learn more about the software, read the "Using the Software Display" chapter and then other chapters that pertain to the tasks you want to perform. See the table of contents for page numbers. ▲

Processing Spectra

This chapter explains how to process spectra you have collected or opened. You can correct the baseline of a spectrum, subtract a spectrum from another spectrum, or smooth a spectrum to improve its appearance.

Unlike “analyzing” a spectrum, explained in the next chapter, “processing” a spectrum changes the actual spectral data. Since your spectral data is important to your work, Encompass provides a way to reverse a change if you make a mistake. See the next section for details.

Undoing a change



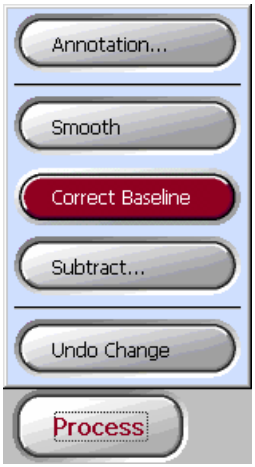
If you have just used Annotation, Smooth or Correct Baseline available through the Process button to change a spectrum and would like to reverse the change, use the Undo Change command available through the Process button. Only the most recent change can be reversed.

Follow these instructions to use Undo Change:

Click the Process button and then choose Undo Change from the menu.

The spectrum is restored to its former state.

Correcting a baseline

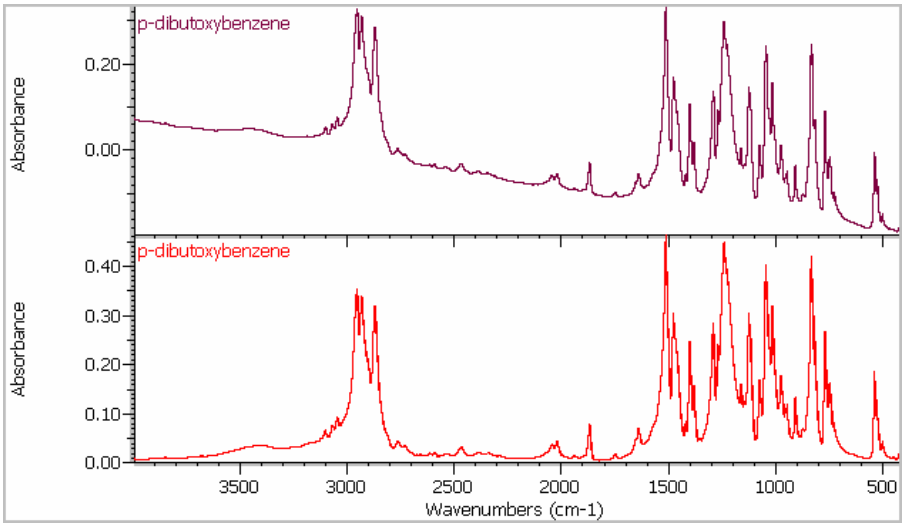


Use the Correct Baseline command available through the Process button to correct the baseline of a spectrum. A baseline consists of those portions of a spectrum where there are no significant absorptions.

Ideally the intensity in these portions of the spectrum is zero absorbance units (or 100% transmittance). In reality baselines may be tilted, shifted or curved. This can be due to the way the sample was prepared, problems with system alignment, or characteristics of the sample material itself.

To correct a baseline, the software uses a special algorithm to calculate values to subtract from the Y values of the data points in the spectrum.

The following illustration shows a spectrum before and after the tilted baseline was corrected.



Notice that the corrected baseline is flat and at zero absorbance units.

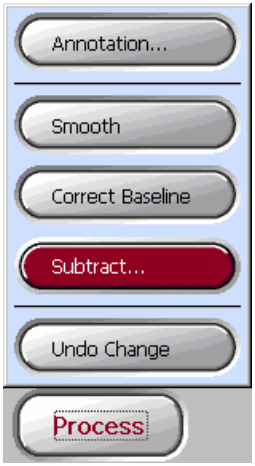
You can obtain better results from searching spectral libraries, subtracting spectra or finding peaks if you first correct the baselines of your spectra. A flat baseline is also helpful when you are visually comparing spectra.

Follow these instructions to correct the baseline of the selected spectrum:

Click the Process button and then choose Correct Baseline from the menu.

The corrected spectrum appears in the spectral display, replacing the original spectrum.

Subtracting a spectrum



Use the Subtract command available through the Process button to subtract a spectrum from the selected spectrum. For each data point, the software calculates the difference in Y value between the two spectra. The resulting spectrum is a plot of these differences across the X-axis range of the original spectra.

Here is how subtraction works: 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 10% component A and 90% component B. Multiplying a reference spectrum of component B by a “subtraction factor” during the subtraction process can make the peak intensities match those in the mixture spectrum. This allows the peaks due to component B to be cleanly subtracted out, leaving only peaks due to component A.

Consider this example: You have used a fixed-pathlength accessory 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 accessory so that you can subtract the reference spectrum from the sample spectrum to produce a spectrum of the compound alone. If you were to subtract the spectra using a subtraction factor of 1 instead of the appropriate factor, the result would exhibit overcompensation for the solvent peaks (giving negative peaks). This is because the “reference” is 100% solvent while the “sample” is only 90% solvent. To achieve a “clean” subtraction, you use a subtraction factor of 0.9 to scale the reference spectrum to 90%.

Algebraically, the subtraction works like this:

Sample - Reference * Factor = Result

To determine the optimum subtraction factor, watch the changes in the common peaks that occur when 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 that produces nulled (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. There will be no negative peaks from the subtracted component.

When to use 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 one 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.

- 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

Tips for using subtraction

Consider these tips when performing a subtraction or evaluating subtraction results:

- Use a subtraction factor that lets you subtract the unwanted component absorptions without subtracting other important spectral information.

- When you subtract the spectrum of a pure reference material from that of a mixture, the peaks may not subtract cleanly. This is because the reference spectrum does not account for any changes that may occur due to molecular interactions with the other components in the mixture or differences in relative concentrations of components. These conditions may cause some peaks to shift slightly or change shape.

How to subtract a spectrum

Follow these steps to subtract one spectrum from another:

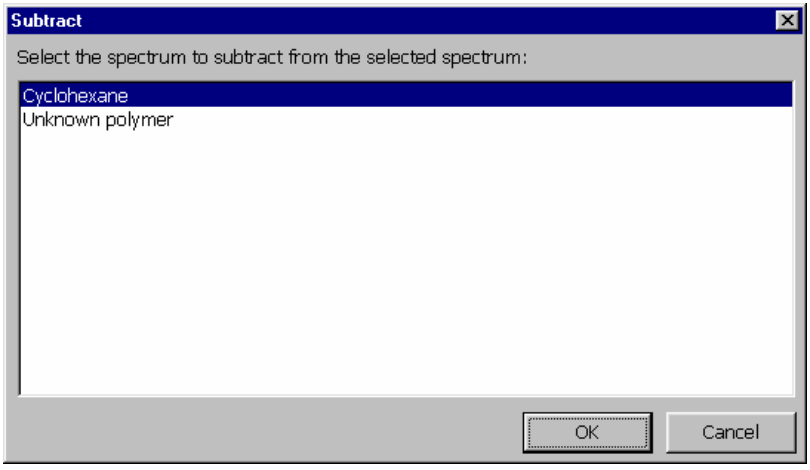
1. **Click the displayed spectrum from which you want to subtract another displayed spectrum.**

   At least two spectra must be displayed when you use this command.

2. **Click the Process button and then choose Subtract from the menu.**

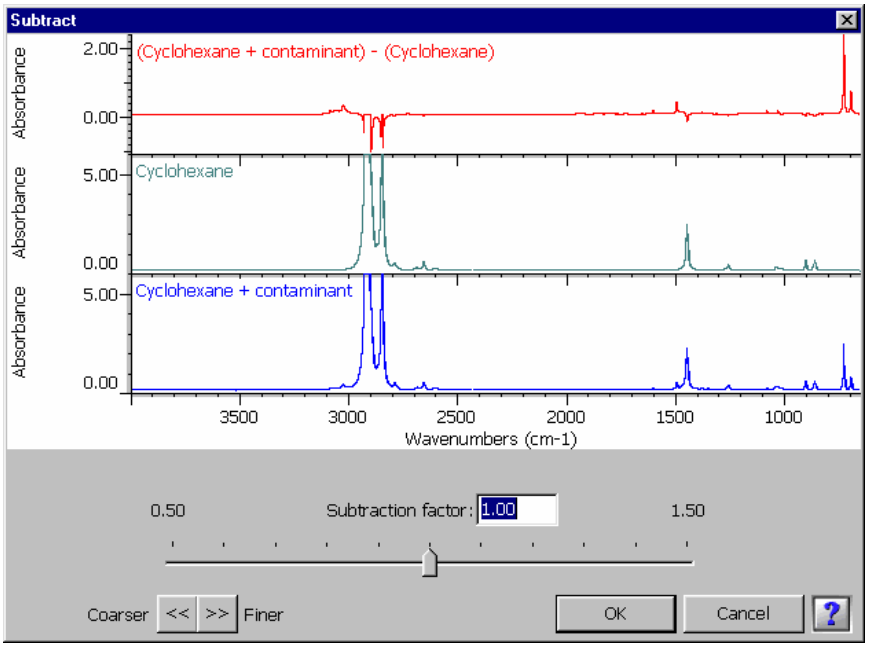
   - If only two spectra are displayed, the Subtract window appears (shown later in this step).

   - If more than two spectra are displayed, a dialog box lists the spectra that have the same resolution as the selected spectrum. Here is an example:



   Click the title of the spectrum you want to subtract and then choose OK. The Subtract window appears.

In the Subtract window the result spectrum appears at the top, with the spectrum being subtracted below it, and the other spectrum at the bottom.



Note You can zoom in on an area of interest in any of the spectra by drawing a box around the area and clicking inside the box, just as you would in the spectral display of the Encompass window. This can be useful when you are trying to “subtract out” a small peak. ▲

The subtraction factor appears below the spectra.

3. Adjust the subtraction factor as desired.

You can type a factor in the Subtraction Factor text box or drag the marker along the Subtraction Factor gauge. If you have a Nicolet IR100, click inside the text box to display the software keyboard.

To change the range of the gauge, use the Coarser and Finer arrow buttons. Each time you click 

, the range is doubled and changes you then make to the subtraction factor by dragging the marker will be twice as large. Each time you click 

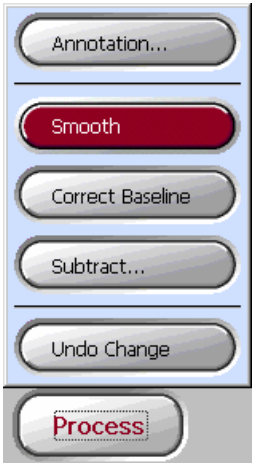
, the range is reduced by one-half and changes you make to the factor will be half as large.

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

   Choose Cancel if you want to cancel the operation.

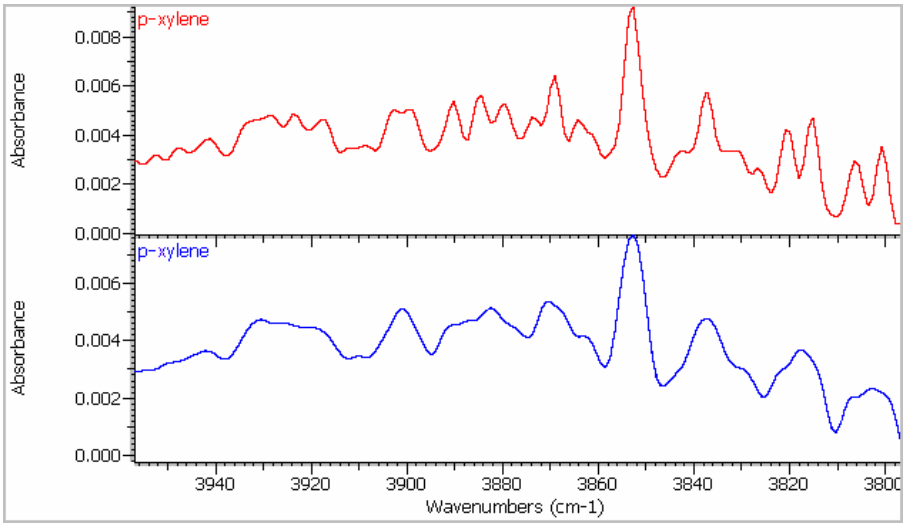
   If you choose OK, the subtraction result spectrum appears in the spectral display. Its title indicates which spectra were used in the subtraction operation. For example, if you were to subtract a spectrum titled “Reference” from a spectrum titled “Mixture,” the title of the result spectrum would be “(Mixture) - (Reference).” You can change the title if desired by using the Information button. See “Viewing information about a spectrum” in the “Using the Software Display” chapter for more information.

Smoothing a spectrum



Use the Smooth command available through the Process button to improve the appearance of a spectrum by preferentially smoothing the jagged or rough features of the spectral data. Smoothing is useful for improving the appearance of peaks obscured by noise.

The following illustration shows a region of a spectrum before smoothing and, below it, the same region after smoothing.



Follow these instructions to smooth the selected spectrum:

Click the Process button and then choose Smooth from the menu.

The smoothed spectrum appears in the spectral display, replacing the original spectrum.

You can further smooth the spectrum by repeating the operation.

Analyzing Spectra

This chapter explains how to analyze spectra you have collected or opened. You can find information about peaks in a spectrum, compare displayed spectra to determine how similar they are, and identify a material by searching its spectrum against a spectral library.

Unlike “processing” a spectrum, explained in the preceding chapter, “analyzing” a spectrum does not change the actual spectral data. After you use a command available through the Analyze button, your spectrum remains in its original form, ready to be used in other operations.

Finding peaks

Use the Find Peaks command available through the Analyze button to find the X-axis locations of peaks in a spectrum, along with the heights of the peaks. The peaks that are found are determined by three criteria that you specify: the threshold, the sensitivity and the spectral region.

The threshold line is a line above which peaks will be found. (In a % transmittance spectrum, it is a line below which peaks will be found.) You can specify the length, location and slope of the line. The X values of its endpoints define the limits of the spectral region within which peaks will be found.

The sensitivity determines how readily small peaks and shoulders on peaks are found. 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.

By adjusting the threshold and sensitivity, you can find the spectral features you are interested in without finding noise and other unimportant features.

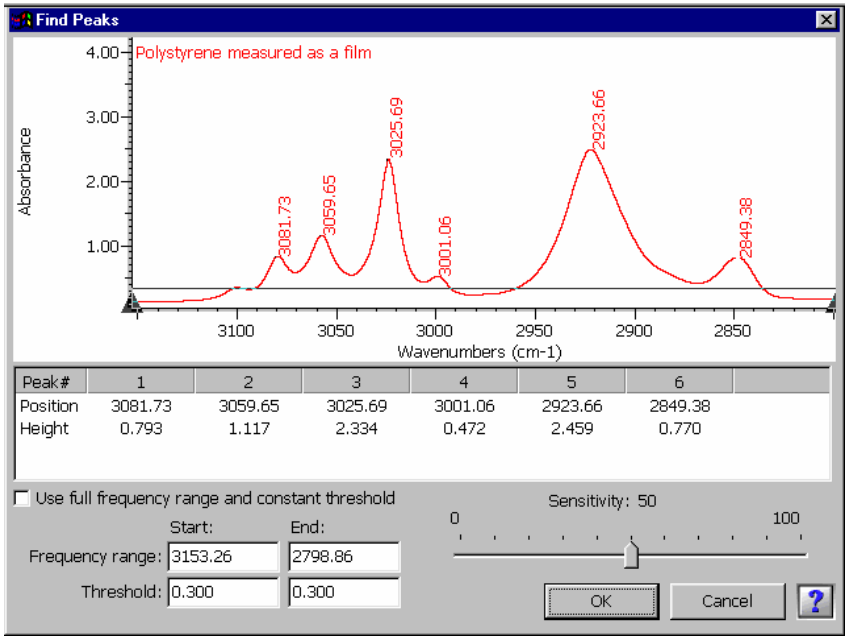
Follow these steps to find the locations of peaks in the selected spectrum:

1. **If desired, zoom in on the area in which you want to find peaks.**

   This can help when you are making fine adjustments to the threshold and sensitivity. See “Zooming in on a spectrum” in the “Using the Software Display” chapter earlier in this manual if you need help.

2. **Click the Analyze button and then choose Find Peaks from the menu.**

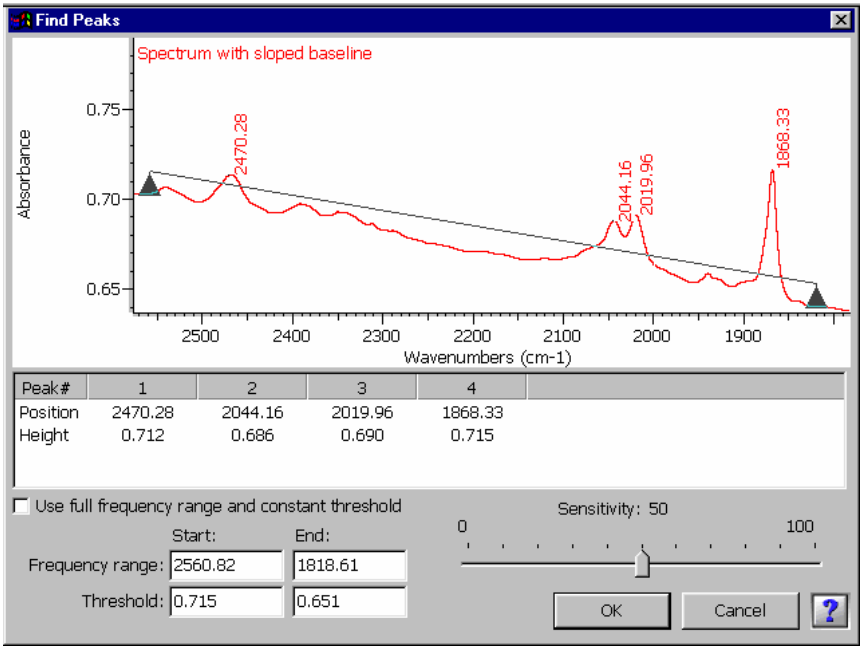
   The Find Peaks window appears showing the spectrum:



Peaks that are higher than the threshold line (at 0.3 absorbance unit in this example) are labeled with their X values and listed in the table below the spectral display. (In a % transmittance spectrum, peaks that are below this line are labeled and listed.) For each found peak, the wavenumber position and peak height are given in the table. If needed, a scroll bar appears at the bottom to let you scroll information into view.

3. **If you want to find peaks across the entire spectrum, using a single threshold value, turn on Use Full Frequency Range And Constant Threshold. If you want to find peaks within just a particular spectral region, or using a sloped threshold line, turn the option off.**

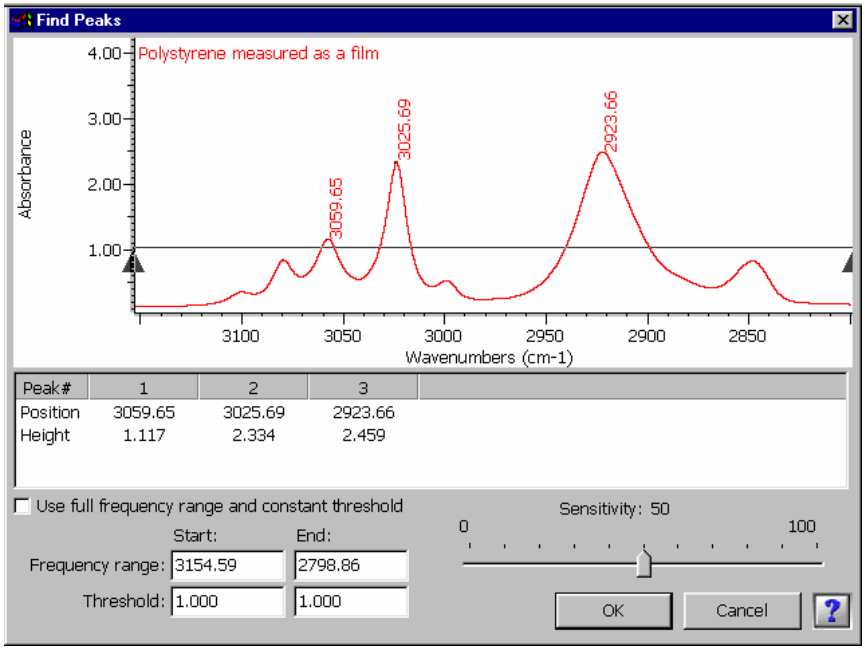
   Using a sloped threshold line is useful for finding peaks that occur along a sloped baseline. By adjusting the threshold line so that it is approximately parallel to the baseline, you can find the peaks without crossing through the baseline. Here is an example:



If you selected Use Full Frequency Range And Constant Threshold, go to the next step. If you turned the option off, go to step 5.

4. **To change the threshold, click above or below the threshold line, or type the desired Y value in the Threshold text box.**

The threshold line moves to the level you clicked, and the new threshold value appears in the Threshold text box. The peaks above the new threshold are labeled with their X values and listed in the table. (In a % transmittance spectrum, peaks below the new threshold are labeled and listed.) Here is our example from step 2 with its threshold line raised to 1.0 absorbance unit:



Notice that fewer peaks are labeled since fewer peaks are above the new threshold.

Go to step 6.

5. **If the Use Full Frequency Range And Constant Threshold option is turned off, position the threshold line.**

   You can drag the triangular endpoints of the line until it has the desired length, location and slope. The values in the Frequency Range and Threshold text boxes are updated automatically to reflect the new line.

Note Once you establish the length, X limits and slope of the line, you can move it up or down by clicking above or below it. ▲

You can also type values in the text boxes. To specify the spectral region within which to find peaks, type the starting and ending X values in the Frequency Range text boxes. This determines the X values of the endpoints of the threshold line. To specify the threshold (Y) values of the endpoints of the line, type the starting and ending Y values in the Threshold text boxes. The threshold line is redrawn to reflect the values you entered.

The peaks above the new threshold are labeled with their X values and listed in the table. (In a % transmittance spectrum, peaks below the new threshold are labeled and listed.)

See the illustration in step 2 for an example.

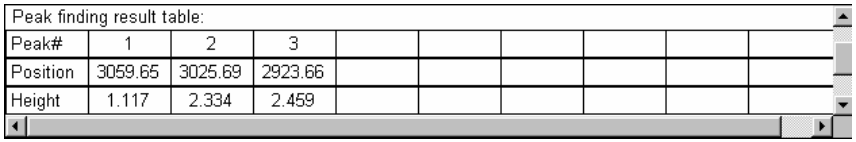
6. **Adjust the sensitivity by dragging the marker along the Sensitivity gauge.**

   The list of found peaks may change as a result.

7. **When you are finished, choose OK to add the results to the report.**

   Choose Cancel if you want to cancel the operation.

   Here is an example showing some peak finding results in the report:



Peak finding result table:

Peak#	1	2	3						
Position	3059.65	3025.69	2923.66						
Height	1.117	2.334	2.459						

   See “About reports” in the “Using the Software Display” chapter for information on displaying and using the report.

   If Show Annotations is selected in the display options, the peak labels appear in the spectral display when you choose OK. See “Displaying annotations” in the “Software Management” chapter for more information.

Note If a label is out of view (for instance, because the peak is very high), you can use Annotation available through the Process button to drag the label to a location where it will be visible within the spectral display. See “Labeling a spectrum” in the “Using the Software Display” chapter for details. ▲

Measuring the height of a peak

Use the Peak Height command available through the Analyze button to measure the height of a peak in a spectrum. The height is measured above a baseline you specify between the low points on either side of the peak and at the X location you specify. (If the spectrum is displayed in % transmittance, the height is measured below a baseline specified between high points on either side of the peak.) Since the height is measured from the baseline rather than from zero absorbance (or 100% transmittance), it is also called the "corrected peak height."

Follow these steps to measure the height of a peak in the selected spectrum:

1. **If desired, zoom in on the peak whose height you want to measure.**

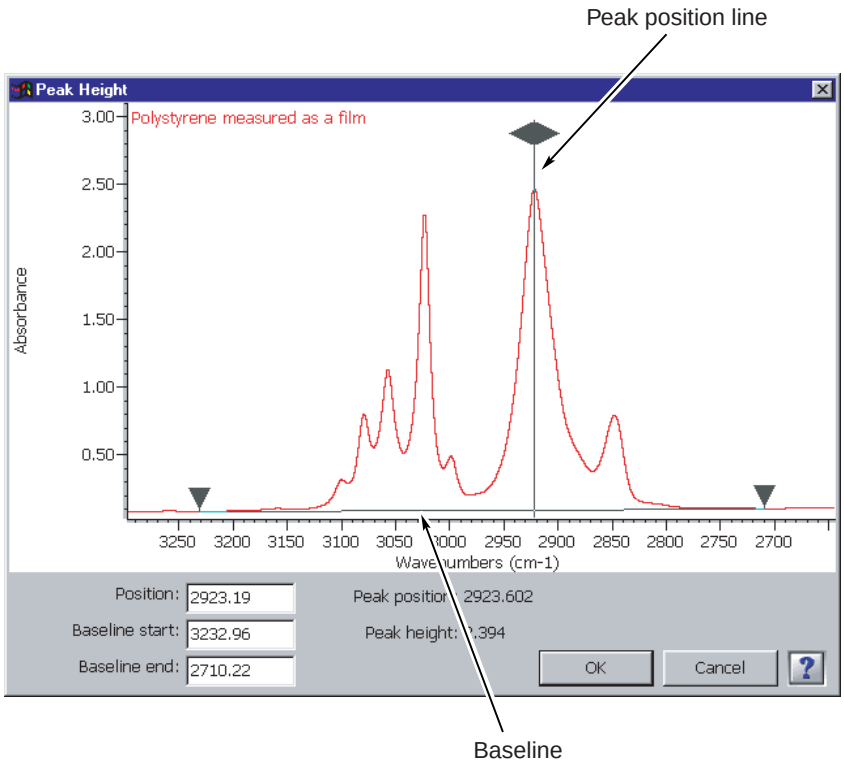
   This can help when you are making fine adjustments to the X-axis position of the area and to the baseline used for the measurement. See "Zooming in on a spectrum" in the "Using the Software Display" chapter earlier in this manual if you need help.

2. **Click the Analyze button and then choose Peak Height from the menu.**

   The Peak Height window appears. Its spectral display contains the spectrum, a vertical line for specifying the X-axis position of the peak, and a horizontal or tilted line connecting two points in the spectrum for specifying a baseline to use for the measurement. (See the illustration in the next step.)

3. **Specify the X-axis position of the peak you want to measure.**

You can drag the vertical line by its diamond-shaped handle to the left or right until the line goes through the top of the peak (bottom of the peak if the spectrum is in % transmittance units). Here is an example:



You can also type an X value in the Position text box. If you have a Nicolet IR100, click inside the text box to display the software keyboard.

4. **Specify the baseline to use for the measurement.**

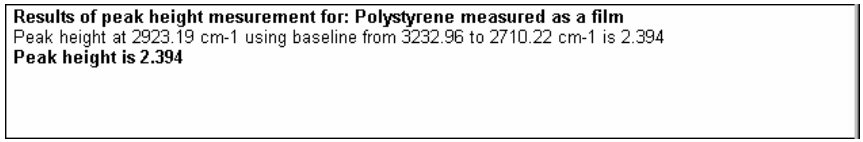
   You can drag the triangular handles of the baseline to the change its endpoints or type starting and ending values in the Baseline Start and Baseline End text boxes, respectively.

   The measured peak height appears below the spectral display.

5. **Choose OK to add the results to the report.**

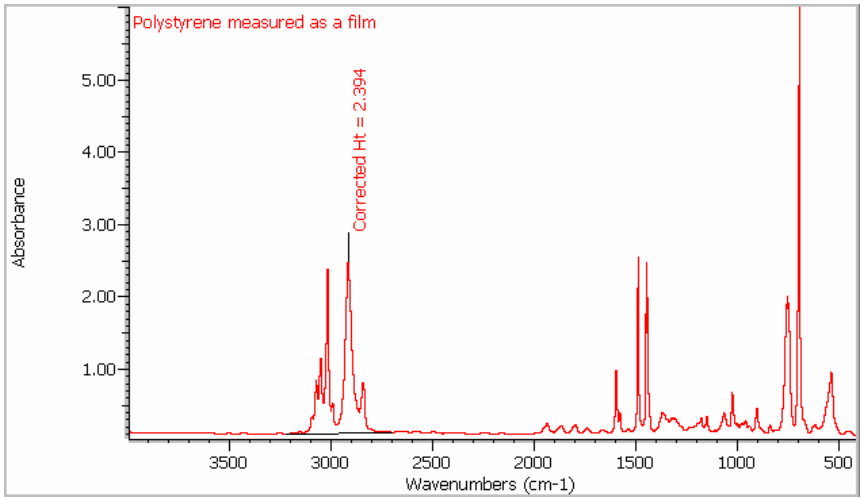
   Choose Cancel if you want to cancel the operation.

   Here is an example showing some peak height measurement results in the report:



   See “About reports” in the “Using the Software Display” chapter for information on displaying and using the report.

If Show Annotations is selected in the display options, the peak height measurement appears in the spectral display when you choose OK. See “Displaying annotations” in the “Software Management” chapter for more information about displaying annotations.

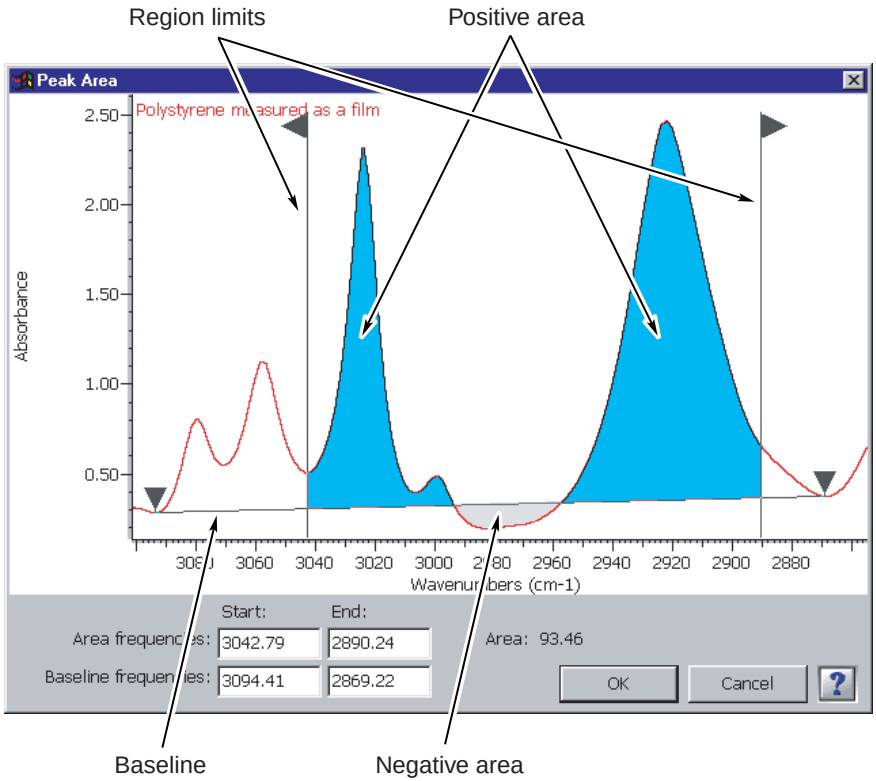


Note If a peak height label is out of view (for instance, because the peak is very high), you can use Annotation available through the Process button to drag the label to a location where it will be visible within the spectral display. See “Labeling a spectrum” in the “Using the Software Display” chapter for details. ▲

Measuring the area of a peak

Use the Peak Area command available through the Analyze button to measure the area of a peak in a spectrum.

The measurement is made on the areas between the spectrum and a baseline you specify, over a specified spectral region. If an area is above the baseline (below the baseline for a % transmittance spectrum), it is considered positive and is shaded light blue in the Peak Area window. If an area is below the baseline (above the baseline for a % transmittance spectrum), it is considered negative and is shaded light gray. Here is an example showing positive and negative areas:



The total area is the sum of all the measured areas. Since the area is measured from the baseline rather than from zero absorbance (or 100% transmittance), it is also called the “corrected peak area.”

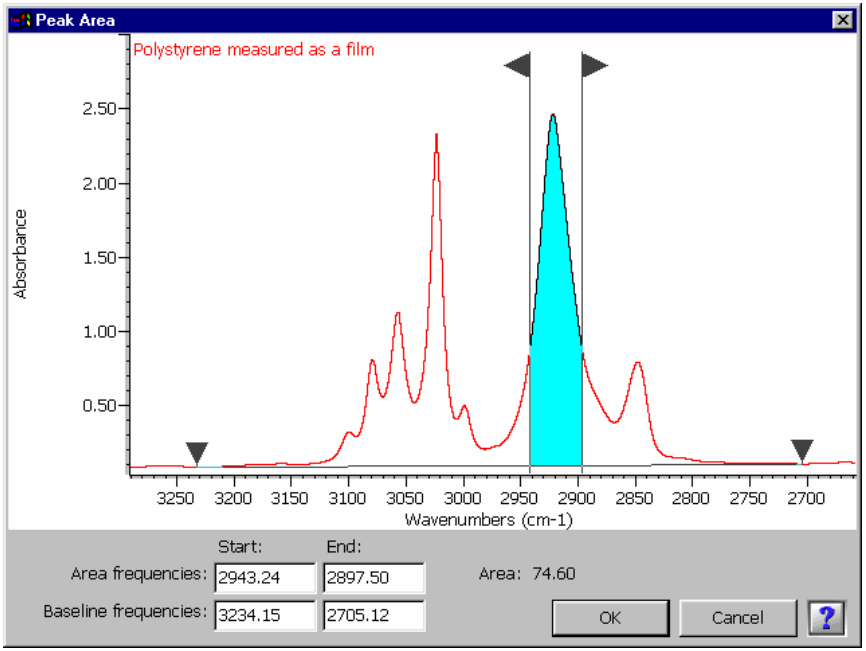
In most cases only a single positive area needs to be measured, as demonstrated in the following procedure:

1. **If desired, zoom in on the peak whose area you want to measure.**

   This can help when you are making fine adjustments to the X-axis limits of the area and to the baseline used for the measurement. See “Zooming in on a spectrum” in the “Using the Software Display” chapter earlier in this manual if you need help.

2. **Click the Analyze button and then choose Peak Area from the menu.**

   The Peak Area window appears. Here is an example:



The two vertical lines specify the X-axis limits of the spectral region to be included in the area measurement. The horizontal or tilted line connecting two points in the spectrum specifies the baseline to be used for the measurement. You can adjust the X-axis limits and the baseline in the next steps.

3. **Specify the X-axis limits of the area you want to measure.**

   You can drag the vertical lines by their triangular handles to the left or right to the desired locations. You can also type X values in the Area Frequencies text boxes. If you have a Nicolet IR100, click inside the text box to display the software keyboard.

4. **Specify the baseline to use for the measurement.**

   You can drag the triangular handles of the baseline to the change its endpoints or type starting and ending values in the Baseline Frequencies text boxes, respectively.

   The measured peak area appears below the spectral display.

5. **Choose OK to add the results to the report.**

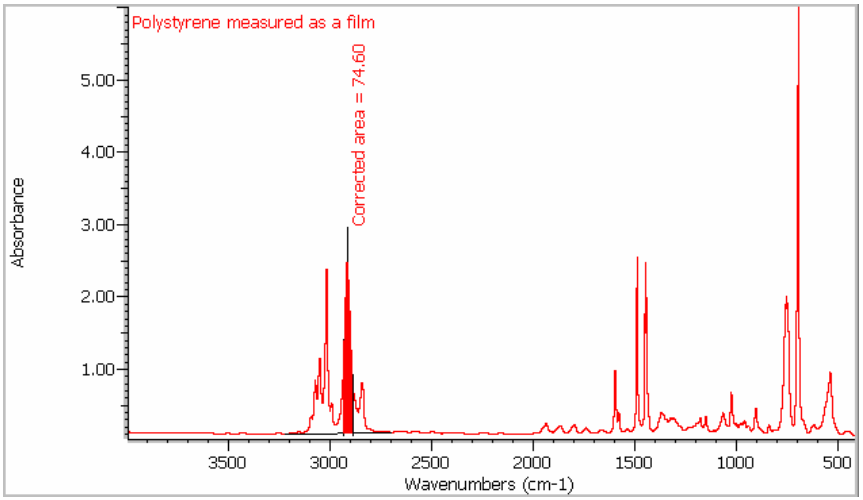
   Choose Cancel if you want to cancel the operation.

   Here is an example showing some peak area measurement results in the report:

Results of peak area measurement for: Polystyrene measured as a film
Peak area from 2943.24 to 2897.50 cm-1 using baseline from 3234.15 to 2705.12 cm-1 is 74.60
Area is 74.60

See “About reports” in the “Using the Software Display” chapter for information on displaying and using the report.

If Show Annotations is selected in the display options, the peak area measurement appears in the spectral display and the peak area is shaded when you choose OK. See “Displaying annotations” in the “Software Management” chapter for more information about displaying annotations.



Note If a peak area label is out of view (for instance, because the peak is very high), you can use Annotation available through the Process button to drag the label to a location where it will be visible within the spectral display. See “Labeling a spectrum” in the “Using the Software Display” chapter for details. ▲

Comparing spectra

Use the Compare command available through the Analyze button to compare the selected spectrum with the other displayed spectra to determine how similar the spectrum is to the others. The comparison is performed using an algorithm you specify. Two choices are available:

The **correlation coefficient** algorithm normally gives the best results when you are comparing spectra that are fairly different. It also removes any effect of offset in the spectra, thus eliminating the effects of baseline variation.

The **Euclidean distance** algorithm normally gives the best results when you are comparing spectra that are fairly similar. It is also less sensitive than the correlation coefficient algorithm to noise. This makes the Euclidean distance algorithm the better choice when you are comparing noisy spectra.

You can also search a spectrum against a library of reference spectra to identify a material. See “Searching a spectral library” later in this chapter for details.

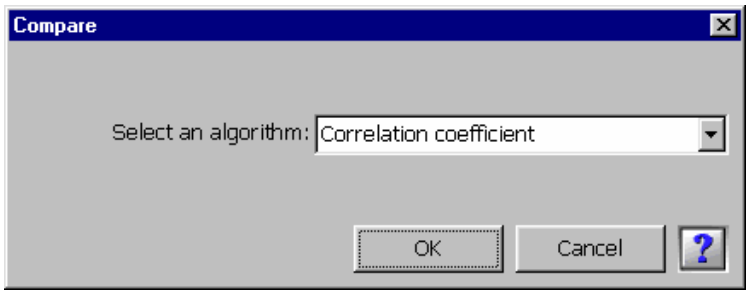
Follow these steps to perform a comparison:

1. **Click the spectrum you want to compare with the other displayed spectra.**

   At least two spectra must be displayed when you use this command.

2. **Click the Analyze button and then choose Compare from the menu.**

   A dialog box prompts you to select an algorithm for the comparison:



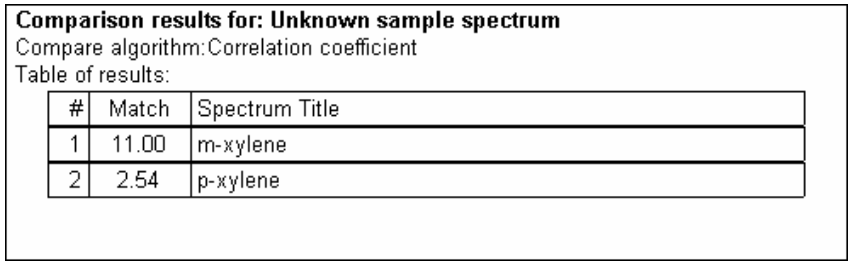
3. **Select the desired algorithm.**

   To do this, click the down arrow button to display a list of available algorithms, and then click the desired algorithm.

4. **Choose OK.**

   A gauge shows the progress of the comparison. (If only a small number of spectra are being compared, the gauge may appear too briefly for you to see it.)

When the comparison is finished, the results appear below the spectral display of the Compare Results window. Here is an example:



Comparison results for: Unknown sample spectrum
Compare algorithm:Correlation coefficient
Table of results:

#	Match	Spectrum Title
1	11.00	m-xylene
2	2.54	p-xylene

The values in the Match column show how similar the selected spectrum is to the other spectra. The higher the value, the more similar the selected spectrum is to the listed spectrum. The highest possible value is 100.

Note You can specify the font for displaying results text by setting Font Name and Font Size in the print options. See “Setting the print options” in the “Software Management” chapter for details. ▲

5. Choose OK to add the results to the report.

Choose Cancel if you want to end the operation without keeping the results.

See “About reports” in the “Using the Software Display” chapter for information on displaying and using the report.

Searching a spectral library

Encompass lets you identify a material by comparing a spectrum of the material with each reference spectrum in a spectral library.

First use the Search Options command available through the Setup button to specify the libraries to search and how to search them. If the desired search option settings have been saved in a configuration, simply open that configuration. See “Opening a configuration” and “Setting the library search options” in the “Software Management” chapter for more information.

Next display the spectral region you want to search. See “Zooming in on a spectrum” or “Zooming out” in the “Using the Software Display” chapter or “Specifying the spectral region to display” in the “Software Management” chapter if you need help.

Then use the Search Library command available through the Analyze button to search the selected spectrum against the specified libraries. The software compares the displayed portion of the spectrum with the corresponding spectral region of each reference spectrum in specified libraries and finds the spectra that most closely match the unknown.

You can also compare a spectrum with other displayed spectra to determine how similar they are. See “Comparing spectra” earlier in this chapter for details.

The Search Results window 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.

Tips for searching a library

Consider the following tips for improving your search results:

- If the baseline of the spectrum is tilted or curved, use the Correct Baseline command available through the Process button to correct the baseline before performing the search. See "Correcting a baseline" in the "Processing Spectra" chapter for details.

- Make sure the signal-to-noise ratio in your sample spectrum is as high as is practical. Since the software regards noise as spectral information, searching a noisy spectrum may give inaccurate results. See "Setting the data collection options" in the "Software Management" chapter for information on how the number of scans, the signal gain and the resolution affect the noise level.

- For best results use the same technique to prepare your samples as was used to prepare the compounds in the libraries being searched.

- You can often obtain better search results by searching spectral regions that exclude totally absorbing bands. These bands have random noise that can adversely affect searches.

How to search a spectral library

Follow these steps to search the selected spectrum against the specified spectral libraries:

1. **If you have a Nicolet IR100 and want to search libraries contained on a flash memory card, insert the card into the flash memory card slot on the front of the spectrometer.**

Important Flash memory cards are sensitive to static electricity. When handling them, always follow the precautions given in "Using flash memory cards" in the "Software Management" chapter. ▲

See "Using flash memory cards" in the "Software Management" chapter for an illustration showing how to insert the card.

2. **Display the spectral region of the spectrum you want to search.**

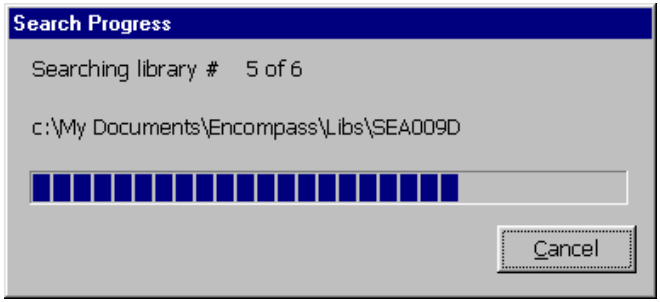
   - If you want to search the region specified in the display options (typically the entire spectrum), choose the Full Display command available through the View button. (To specify the region to display, use the Display Options command available through the Setup button.)

   - If you want to search a region other than the one specified in the display options, display the region by drawing a box around it and then clicking inside the box. (If the region is currently out of view, first expand the display by choosing the Fully Display command available through the View button.)

   See “Zooming in on a spectrum” or “Zooming out” in the “Using the Software Display” chapter or “Specifying the spectral region to display” in the “Software Management” chapter for more information about using the features mentioned above.

3. **Click the Analyze button and then choose Search Library from the menu.**

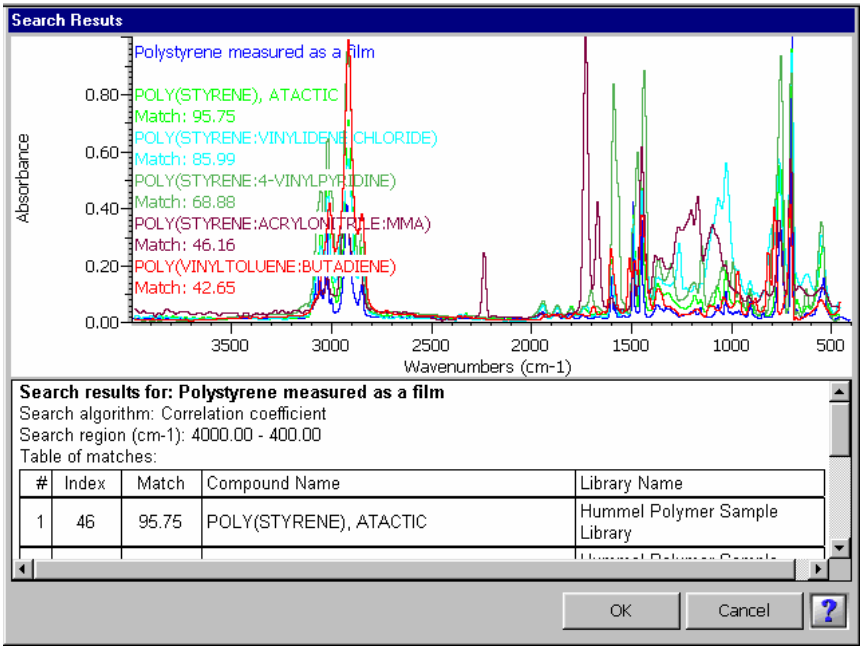
   A gauge shows the progress of the search:



(If not many libraries are being searched and the libraries are small, the gauge may appear too briefly for you to see it.) You can cancel the search by choosing Cancel.

When the search is finished, the results appear in the Search Results window.

Here is an example:



If needed, scroll bars are provided for scrolling information into view.

Note You can specify the font for displaying results text by setting Font Name and Font Size in the print options. See “Setting the print options” in the “Software Management” chapter for details. ▲

4. **Choose OK to add the results to the report and the found library spectra to the spectral display of the Encompass window.**

   Choose Cancel if you want to end the operation without saving the results.

   See “About reports” in the “Using the Software Display” chapter for information on displaying and using the report.

Working with libraries

Use the Library Organizer command available through the Analyze button to perform the library management operations listed below.

- View information about a library and the spectra it contains. You can edit some of the information in a user library. See “Viewing a library.”
- Add a spectrum to a user library. See “Adding a spectrum to a user library.”
- Delete a spectrum from a user library. You can compress the library after deleting a spectrum from it. See “Deleting a spectrum from a user library.”
- Export a library spectrum to the spectral display. See “Exporting a library spectrum.”
- Search a library for spectra whose titles or custom information fields contain specified text. See “Searching a library for text.”
- Delete a library. See “Deleting a library.”
- Create a user library. See “Creating a user library.”
- Copy a library to a new location (for Nicolet IR100 systems only). See “Copying a library to a new location.”

If Require Log-In is turned on in System Manager and Macro Mode Only or Specified Configurations Only is selected, the Library Organizer is available only to the system administrator. If Require Log-In is turned on and All Menus Available is selected, these buttons in the Library Organizer are available only to the administrator: Info (for libraries), Compress and Delete (for libraries and library spectra). See “Using System Manager” in the “Software Management” chapter and “Starting the software” in the “Getting Started” chapter for more information.

Only libraries that are in OMNIC format can be used in these operations. All libraries that you create with Encompass or purchase from us for use with Encompass are in OMNIC format.

Viewing a library

You can use the Library Organizer command available through the Analyze button to view information about a library and the spectra it contains. You can edit some of the information in a user library. Follow these steps:

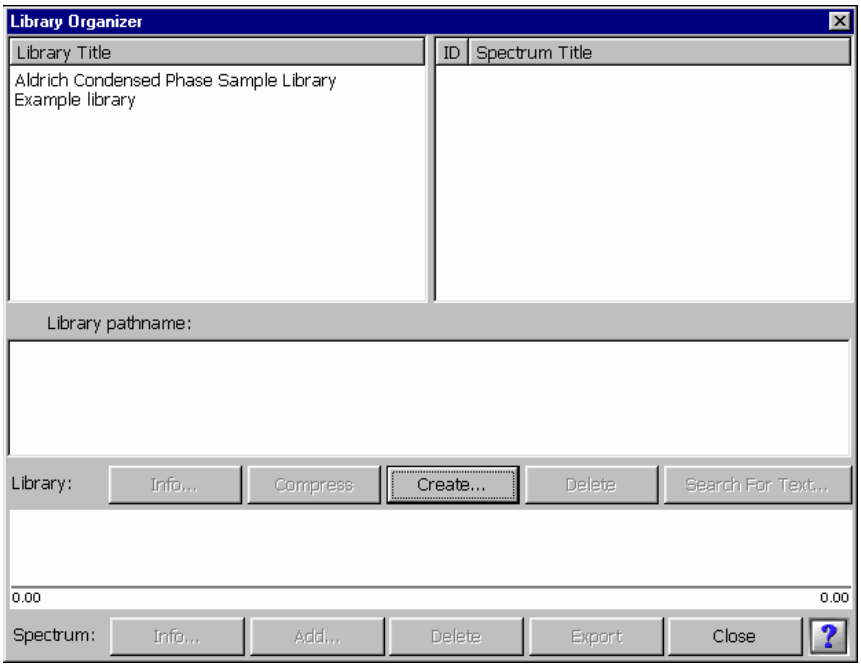
1. **If you have a Nicolet IR100 and want to work with libraries contained on a flash memory card, insert the card into the flash memory card slot on the front of the spectrometer.**

Important Flash memory cards are sensitive to static electricity. When handling them, always follow the precautions given in "Using flash memory cards" in the "Software Management" chapter. ▲

See "Using flash memory cards" in the "Software Management" chapter for an illustration showing how to insert the card.

2. **Click the Analyze button and then choose Library Organizer from the menu.**

   The Library Organizer appears:



   The appearance of this dialog box varies slightly depending on the model spectrometer you have.

   The titles of the available libraries are listed near the upper-left corner. Scroll bars are provided when needed to scroll titles into view.

3. **Click the title of the library you want to view.**

The pathname (directory location and filename) of the selected library appears below the list of libraries (see the following illustration). The identification (ID) numbers and titles of the spectra contained in the library appear in the box to the right. The ID numbers indicate the order in which the spectra were added to the library.

Below the pathname is information about the selected library.

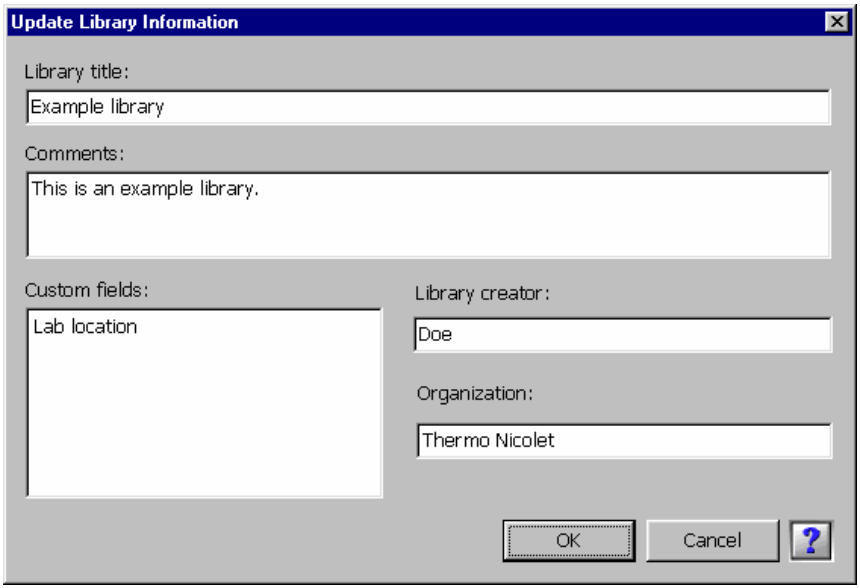
The information is grouped in folders named for the kind of information they contain. To open a closed folder, double-click it.

If a piece of information is next to a lock icon bearing a green check mark, you can edit the information by using the Info button (explained later in this step).

If a piece of information is next to a lock icon bearing a red “X,” the information cannot be edited. This is the case for all the information in a commercial library.

Scroll bars are provided when needed to scroll information into view.

If you are viewing a user library and want to edit the library information, click the Info button in the row of buttons labeled "Library." (The button is available only for user libraries and only if you have logged in as the system administrator.) The Update Library Information dialog box appears showing the information that can be edited:

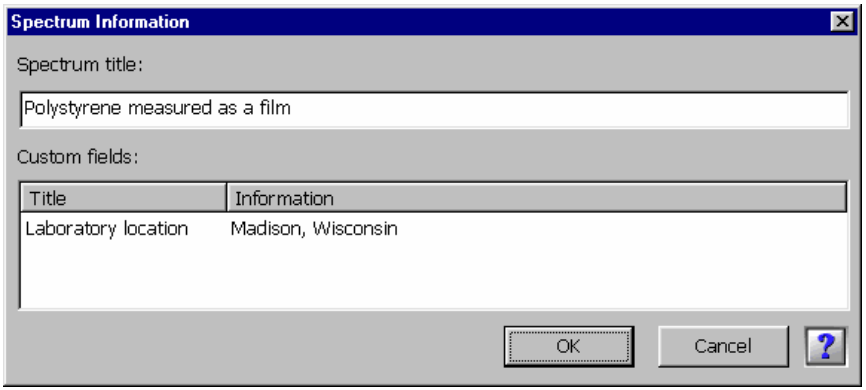


Change the information as desired by typing in the text boxes and then choose OK. If you have a Nicolet IR100, click inside a text box to display the software keyboard.

4. **To see information about a library spectrum, click the spectrum in the list in the upper-right corner of the dialog box and then click the Info button in the row of buttons labeled "Spectrum."**

   When you click the spectrum in the list, an image of the spectrum appears near the bottom of the window.

   When you click the Info button, the Spectrum Information dialog box dialog box appears. Here is an example:



   If the spectrum is in a user library, you can edit the information. To change the spectrum title, type the desired title in the Spectrum Title text box. If you have a Nicolet IR100, click inside the text box to display the software keyboard. To change the information in a custom field, type the desired information in the appropriate row in the Information column of the table.

When you are finished, choose OK (or Cancel) if the spectrum is in a user library, or choose Cancel if the spectrum is in a commercial library.

5. **When you are finished viewing the library, choose Close.**

Adding a spectrum to a user library

You can use the Library Organizer command available through the Analyze button to add a spectrum to a user library. See "Deleting a spectrum from a user library" later in this chapter for information on deleting a library spectrum.

Note You cannot add a spectrum that was exported from a commercial library. See "Exporting a library spectrum" later in this chapter for information on exporting library spectra. ▲

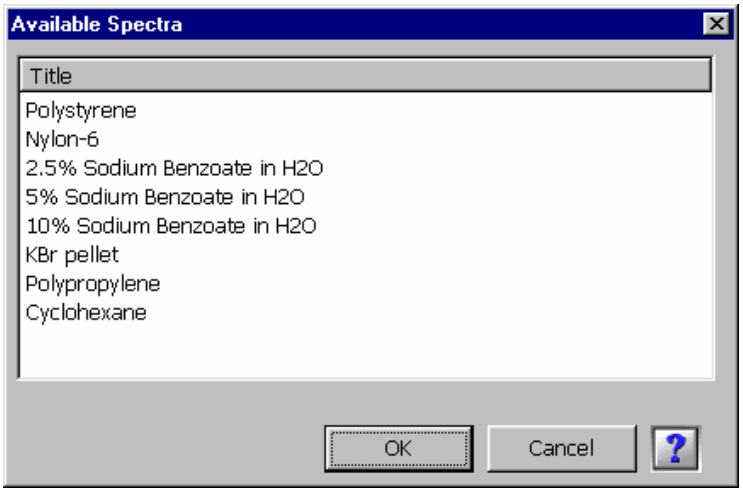
Follow these steps to add a user library spectrum:

1. **In the Library Organizer, click the title of the user library to which you want to add a spectrum.**

   For instructions for displaying the Library Organizer, see the first two steps of the procedure in "Viewing a library."

2. **Click the Add button.**

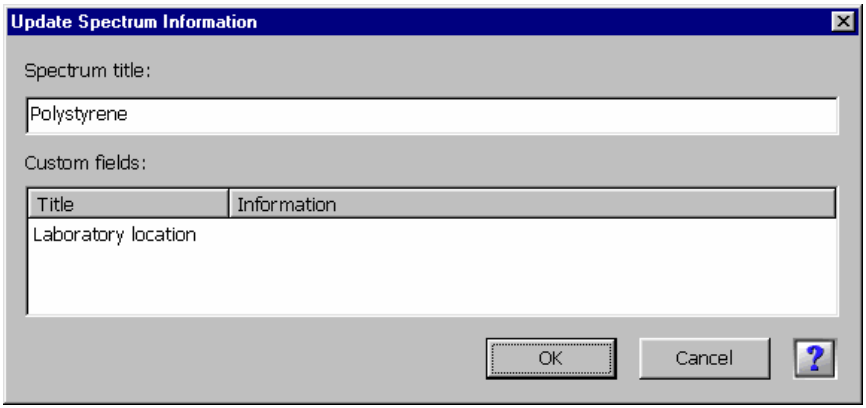
   The Available Spectra dialog box appears listing the currently open spectra, except those that were exported from a commercial library. Here is an example:



3. **Click the title of the spectrum you want to add.**

4. **Choose OK.**

   The Update Spectrum Information dialog box appears:



   You can change the title of the spectrum by typing a new title in the Spectrum Title text box. If you have a Nicolet IR100, click inside the text box to display the software keyboard. To change the information in a custom field, type the desired information in the appropriate row in the Information column of the table.

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

   If you want to add another spectrum to the library, return to step 2. If you are finished using the Library Organizer, go to the next step.

6. **Choose Close to close the Library Organizer.**

Deleting a spectrum from a user library

If you have logged in as the system administrator, you can use the Library Organizer command available through the Analyze button to delete a spectrum from a user library. See “Adding a spectrum to a user library” earlier in this chapter for information on adding a spectrum to a library.

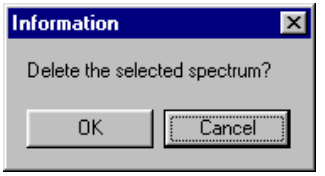
Follow these steps to delete a user library spectrum:

1. **In the Library Organizer, click the title of the user library from which you want to delete a spectrum.**

   For instructions for displaying the Library Organizer, see the first two steps of the procedure in “Viewing a library.”

2. **Click the spectrum you want to delete in the list near the upper-right corner of the Library Organizer and then click the Delete button in the row of buttons labeled “Spectrum.”**

   A message asks you if want to delete the spectrum:



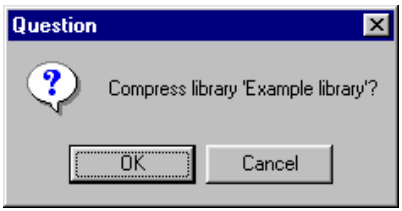
3. **Choose OK.**

4. **If desired, compress the library from which you deleted a spectrum.**

   When you compress a library, the spectra it contains are renumbered consecutively with no gaps due to deleted spectra. As a result, the ID numbers of some of the spectra will change. This process can take several minutes if the library is large.

To compress the library, click its title and then click the Compress button. (The button is available only if you have logged in as the system administrator.)

A message asks whether to compress the library:



Choose OK. A gauge shows the progress of the compression. When the compression is complete, a message informs you:

Choose OK.

If you want to delete another spectrum from the library, return to step 2. If you are finished using the Library Organizer, go to the next step.

5. **Choose Close to close the Library Organizer.**

Exporting a library spectrum

You can use the Library Organizer command available through the Analyze button to export a library spectrum to the spectral display of the Encompass window. You can then perform operations on the spectrum just as you would on a spectrum you have collected or opened.

Note You cannot save a spectrum exported from a commercial library. See "Saving a spectrum or report" in the "Saving Spectra and Reports" chapter for information on saving spectra. ▲

Follow these steps to export a library spectrum:

1. **In the Library Organizer, click the title of the library that contains the spectrum you want to export.**

   For instructions for displaying the Library Organizer, see the first two steps of the procedure in "Viewing a library."

2. **Click the spectrum you want to export in the list near the upper-right corner of the Library Organizer and then choose Export.**

   If you want to export another spectrum in the library, repeat this step.

3. **Choose Close the close the Library Organizer.**

   The exported spectra are displayed in the spectral display of the Encompass window.

Searching a library for text

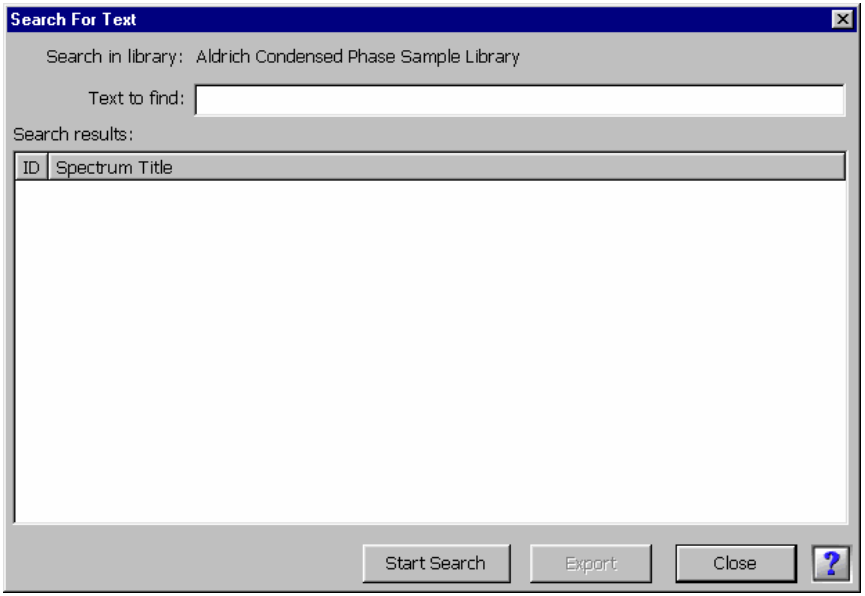
You can use the Library Organizer command available through the Analyze button to search a library for spectra whose titles or custom information fields contain specified text. Follow these steps:

1. **In the Library Organizer, click the title of the library you want to search.**

   For instructions for displaying the Library Organizer, see the first two steps of the procedure in “Viewing a library.”

2. **Click the Search For Text button.**

   The Search For Text dialog box appears.

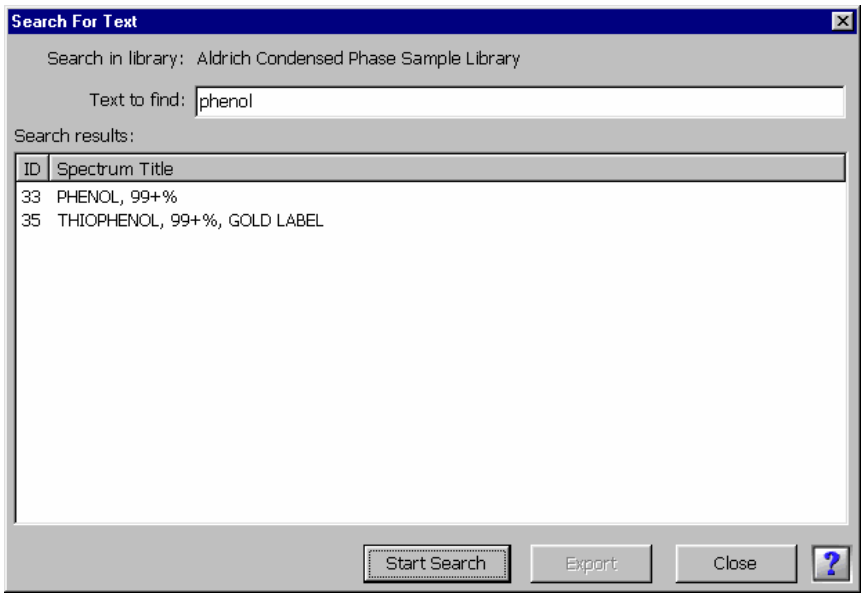


3. **Type the text you want to find in the Text To Find text box.**

   If you have a Nicolet IR100, click inside the text box to display the software keyboard.

4. **Click the Start Search button.**

   The found library spectra are listed in the Search Results box. Here is an example:



5. **If you want to display a found spectrum in the spectral display of the Encompass window, click the spectrum's title and then choose Export.**

   To export another found spectrum, repeat this step.

6. **If you want to search for other text, return to step 3; otherwise, choose Close.**

7. **Choose Close the close the Library Organizer.**

   Any spectra you exported appear in the spectral display.

Deleting a library

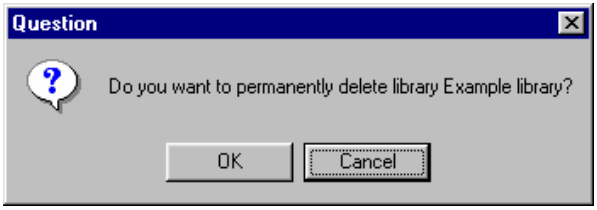
If you have logged in as the system administrator, you can use the Library Organizer command available through the Analyze button to delete a library. Follow these steps:

1. **In the Library Organizer, click the title of the library you want to delete.**

   For instructions for displaying the Library Organizer, see the first two steps of the procedure in “Viewing a library.”

2. **Click the Delete button in the row of buttons labeled “Library.”**

   A message asks whether to delete the library. Here is an example:



3. **Choose OK.**

   Choose Cancel if you want to cancel the operation.

   If you choose OK, the library is deleted.

4. **Choose Close the close the Library Organizer.**

Creating a user library

You can use the Library Organizer command available through the Analyze button to create a user library to which you can add your own spectra. You can later search the library just as you would a commercial library to identify an unknown spectrum. See “Adding a spectrum to a user library” and “Searching a spectral library” earlier in this chapter for more information.

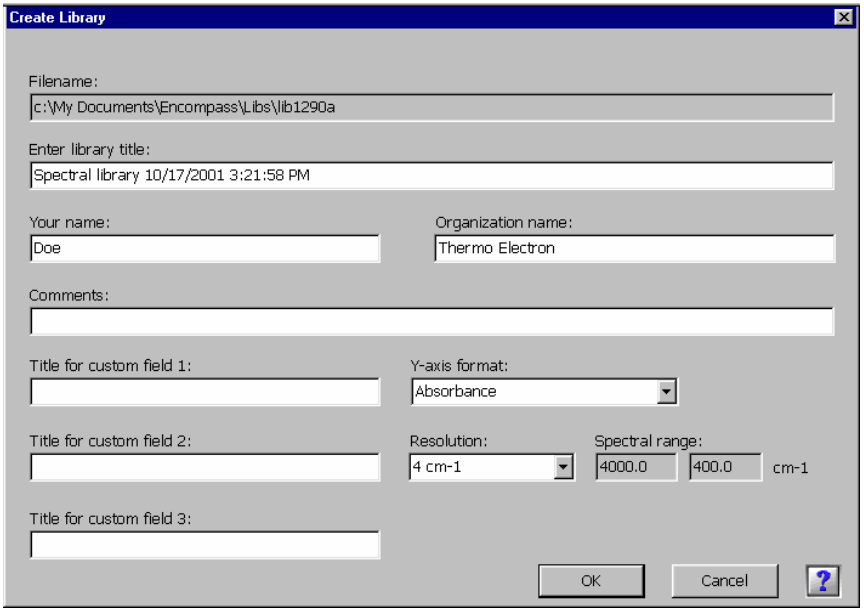
Follow these steps to create a user library:

1. **Click the Analyze button and then choose Library Organizer from the menu.**

   The Library Organizer appears.

2. **Click the Create button.**

   The Create Library dialog box appears:



The filename that will be used for the new library is automatically assigned and appears in the Filename box.

The spectral range limits of the new library appear in the Spectral Range boxes.

3. **Type a title for the library in the Enter Library Title text box.**

   If you have a Nicolet IR100, click inside the text box to display the software keyboard.

4. **Type your name in the Enter Your Name text box, and type the name of your organization in the Organization Name text box.**

5. **If you want to include any comments about the library, type them in the Comments text box.**

6. **If you want to include any custom information fields, type a title for each field.**

   When you later add spectra to the library, you can enter information in the fields. Use these fields for entering product names or lot numbers, the location of a laboratory, or any other information that would be useful.

   Type the titles for the first through third fields in the Title For Custom Field 1, 2 and 3 text boxes, respectively.

7. **Use Y-Axis Format to specify the Y-axis units for the library spectra.**

   Click the down arrow button to display a list of available units, and then click the desired units.

8. **Select a resolution for the library spectra from the Resolution drop-down list box.**

   Click the down arrow button to display a list of available settings, and then click the desired setting.

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

10. **When you are finished using the Library Organizer, choose Close.**

    If you have a Nicolet IR100 and want to store the new library on a flash memory card, follow the instructions in the next section, "Copying a library to a new location."

Copying a library to a new location

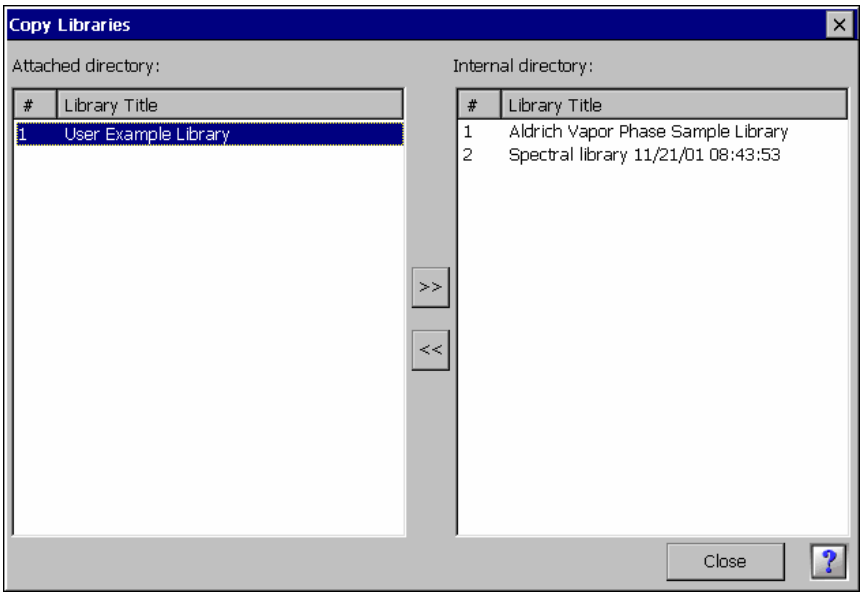
If you have a Nicolet IR100, you can use the Library Organizer command available through the Analyze button to copy a library to a different location. This is useful for backing up libraries onto a flash memory card or moving libraries you have purchased on a flash memory card. You can also use this feature if you have run out of room in internal flash memory and need to move a library to an external flash memory card.

Follow these steps:

1. **In the Library Organizer, click the Copy button**

   For instructions for displaying the Library Organizer, see the first two steps of the procedure in "Viewing a library."

When you click the Copy button, the Copy Libraries dialog box appears. Here is an example:



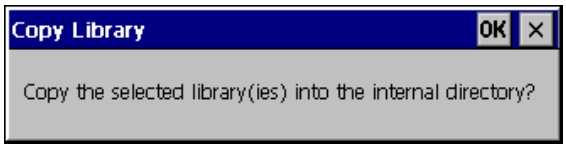
The libraries contained on the external flash memory card are listed in the Attached Directory box. The libraries contained in the internal flash memory are listed in the Internal Directory box.

2. **Click the title of the library you want to copy.**

3. **Click the appropriate arrow button to copy the library.**

   To copy a library from the external flash memory card to the internal flash memory, click >>. To copy a library from the internal flash memory to the external flash memory card, click <<.

A message asks whether to copy the library. Here is an example:

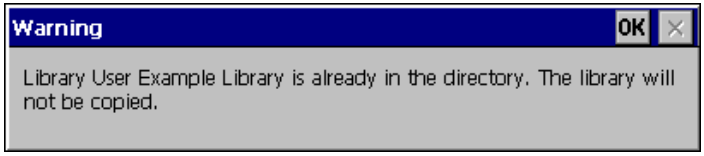


4. **Choose OK.**

   Choose Cancel if you don't want to copy the library.

   The copied library is listed in the new location.

   If the library you are attempting to copy is already in that location, a message informs you. Here is an example:

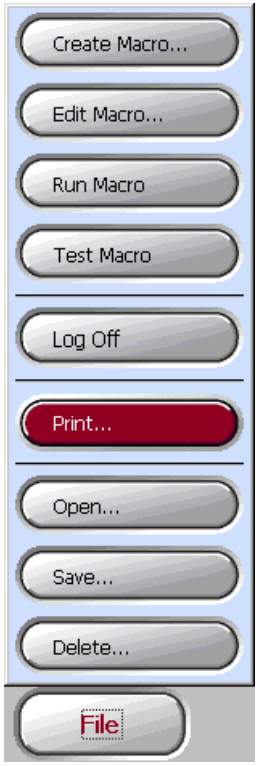


   Choose OK.

   Repeat steps 2 through 4 for any additional libraries you want to copy.

5. **When you are finished copying libraries, choose Close.**

Printing Spectra and Reports



Use the Print command available through the File button to print spectra and reports displayed in the Encompass window. For information on setting options that affect printing, see “Setting the print options” in the “Software Management” chapter. For information about reports see “About reports” in the “Using the Software Display” chapter.

Follow these instructions to print spectra, a report or both:

1. **Click the File button and then choose Print from the menu.**

   The Print dialog box appears.

2. **Set the printer parameters as desired and then choose OK.**

   The items specified in the print options are printed.

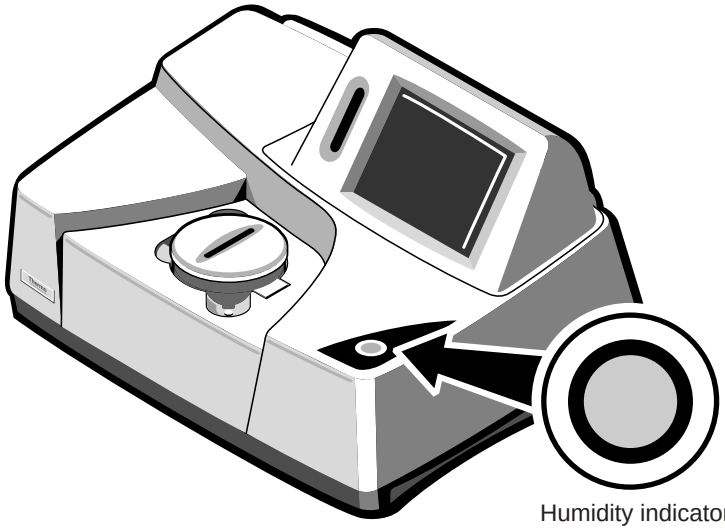
More About Your Spectrometer

This chapter explains how to check the desiccant inside your spectrometer and purge the spectrometer. It also discusses aligning the spectrometer's interferometer.

Checking the desiccant

Your spectrometer contains a container of desiccant that keeps the optics compartment free of water vapor. This protects the beamsplitter and other optical components from moisture damage. You should check the desiccant weekly, as explained below.

The humidity indicator shows whether the desiccant is still active.



Humidity indicator

If the indicator is blue, the desiccant is still effective. If the indicator has turned white or pink, the desiccant is no longer effective and must be replaced or dried. See “Replacing the desiccant canister” in the “Servicing Your Spectrometer” chapter of the manual titled *Servicing Your Spectrometer* for instructions.

Important Replace or dry the desiccant when the indicator begins to change from blue to white, before it turns pink. Failure to replace or dry the desiccant soon enough can damage the KBr beamsplitter in your spectrometer. ▲

Purging the spectrometer

A spectrometer can be purged with a nonreactive gas to minimize the amount of water vapor and carbon dioxide inside. If the level of either of these two gases is too high, absorptions of infrared energy by the gas will cause unwanted peaks that may obscure the peaks due to the sample. Also, if the background spectrum contains more water vapor or carbon dioxide absorption than does the sample spectrum, negative peaks will result.

⚠ Warning *Never* use a flammable gas, argon or helium to purge the spectrometer. The purge gas must be free of moisture, oil, carbon dioxide and other reactive or infrared-absorbing materials. We recommend using dry air supplied by a purge gas generator or pure air generator (available from us), or dry nitrogen. ▲

Important If you use chlorinated solvents, perfluorochlorinated solvents, or solvents containing halogenated hydrocarbons (for example, Freon®), you must purge the spectrometer. The interaction of these solvents with an IR source can corrode spectrometer components. Do not expose the spectrometer to these solvents any longer than necessary. Optical damage caused by failure to purge the spectrometer is not covered under your warranty. ▲

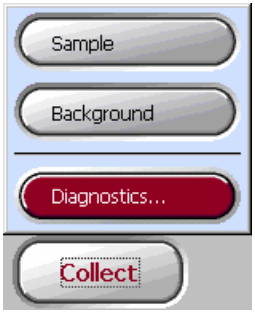
If your spectrometer is purged, keep the purge gas flow rate between 10 and 35 cubic feet per hour. See “Connecting purge gas lines” in the “Installing Your Spectrometer” chapter of the manual titled *Installing Your Spectrometer* for information on connecting the purge hardware.

Aligning the spectrometer

To ensure optimum system performance (high signal intensity, low noise and good sensitivity), you should occasionally align the spectrometer's interferometer. Perform an alignment after you replace the laser or if performance has deteriorated (the largest peak of an open-beam interferogram has dropped to less than 6 volts). For best performance align the spectrometer at least once a month.

See "Aligning the beamsplitter" in the "Servicing Your Spectrometer" chapter of the manual titled *Servicing Your Spectrometer* for complete alignment instructions.

Diagnostics



This chapter explains how to use the Diagnostics command available through the Collect button to determine the causes of problems that may occur with the spectrometer and to perform other tasks. Also see the “Troubleshooting” chapter, which explains how to solve software and applications problems that could occur while you are using the spectrometer.

If you are unable to solve a problem after following the provided instructions, contact Technical Support.

If you have a Nicolet IR100 (that is not part of a Transport Kit) or a Nicolet IR200 with Encompass software, you can use the Diagnostics command to verify the laser. If you have a Nicolet IR200 with EZ OMNIC software, use the Laser Verification button on the Diagnostic tab of the Experiment Setup dialog box instead. For instructions find “laser” in the OMNIC Help system Index and go to the “How to verify the laser frequency on a Nicolet IR200” topic.

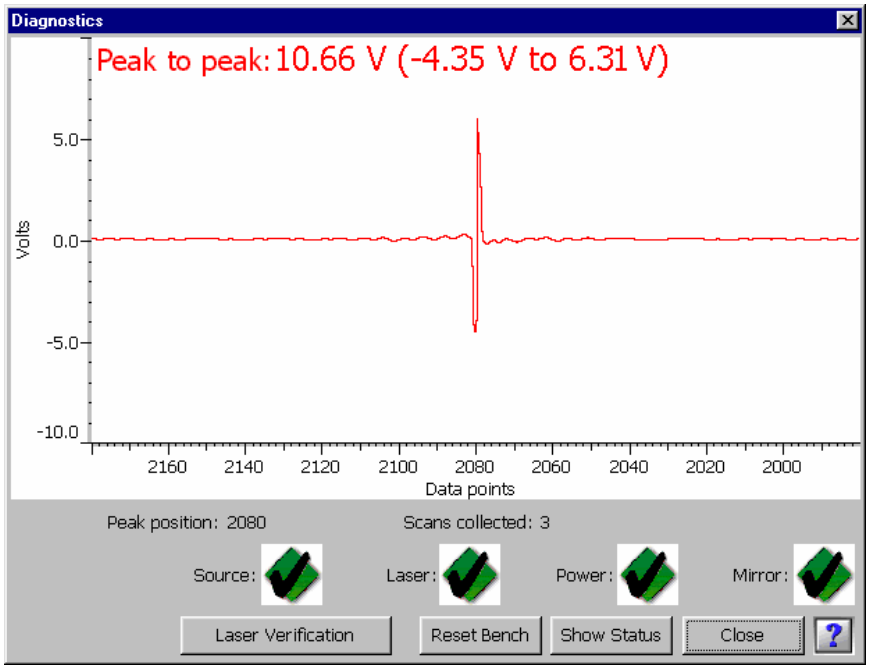
If you have a Transport Kit, you can use the Diagnostics command to adjust the laser amplitude.

The command also provides a button for resetting the spectrometer’s interferometer.

Follow these steps to use the diagnostic features:

1. **Click the Collect button and then choose Diagnostics from the menu.**

   The Diagnostics window appears:



   Use the Reset Bench button only as explained in the "Troubleshooting Your Spectrometer" chapter of *Servicing Your Spectrometer*.

The window contains a live display of the interferogram, the signal produced by the detector. Information about the interferogram peak appears below the live display. This information can be helpful when you are troubleshooting problems. (See the “Troubleshooting” chapter later in this manual for more information.) Normally, the peak-to-peak signal intensity with no sample installed is approximately 8 volts. The intensity may be lower if you are using an accessory.

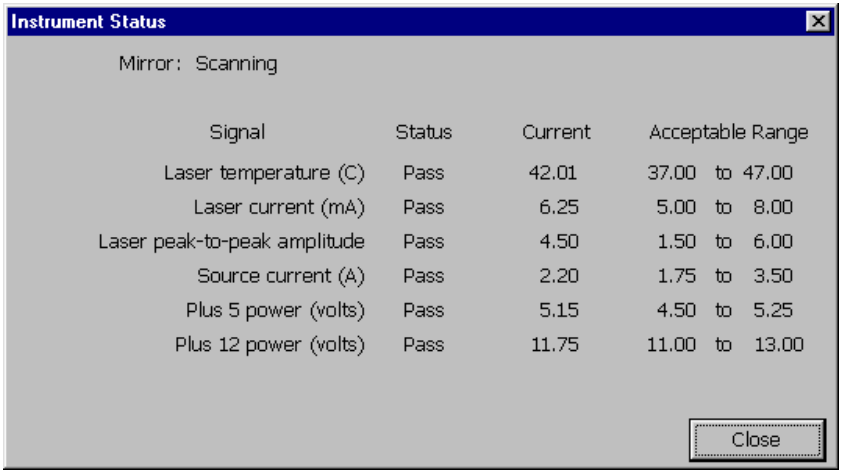
When you choose the Diagnostics command, it automatically performs four tests—on the source, laser, power and moving mirror (a part in the interferometer)—and displays the results. If an item passes a test, a check mark appears to the right of the item name. If an item fails a test, an X appears instead. See “Troubleshooting table” in the “Troubleshooting Your Spectrometer” chapter of the manual titled *Servicing Your Spectrometer* for instructions.

You can also see the numerical results of some diagnostic tests by using the Show Status button, as explained in the next step.

2. **If you want to see the operation status of some spectrometer components, use the Show Status button.**

   The Instrument Status dialog box appears. Here is an example:

The items that appear for your model may differ from those shown in this example.



   For each measured item, the dialog box shows the current measured value and the allowed range of values. If the current value is within the acceptable range, “Pass” appears in the Status column. If the current value is outside the acceptable range, “Fail” appears.

Note The Reference Detector (Volts) item, if available, shows information only in the Current column. ▲

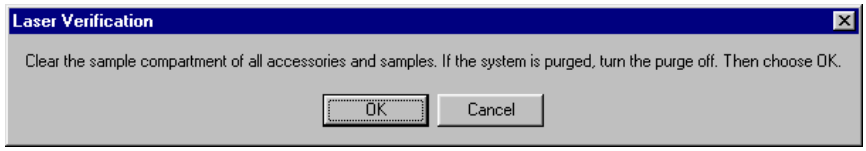
   If you have a Transport Kit and the laser amplitude is outside the acceptable range, use the Laser Verification button to adjust the laser amplitude, as explained in the next step.

   When you are finished viewing the information, choose Close.

3. **If you want to verify the laser, or adjust the laser amplitude on a Transport Kit, use the Laser Verification button.**

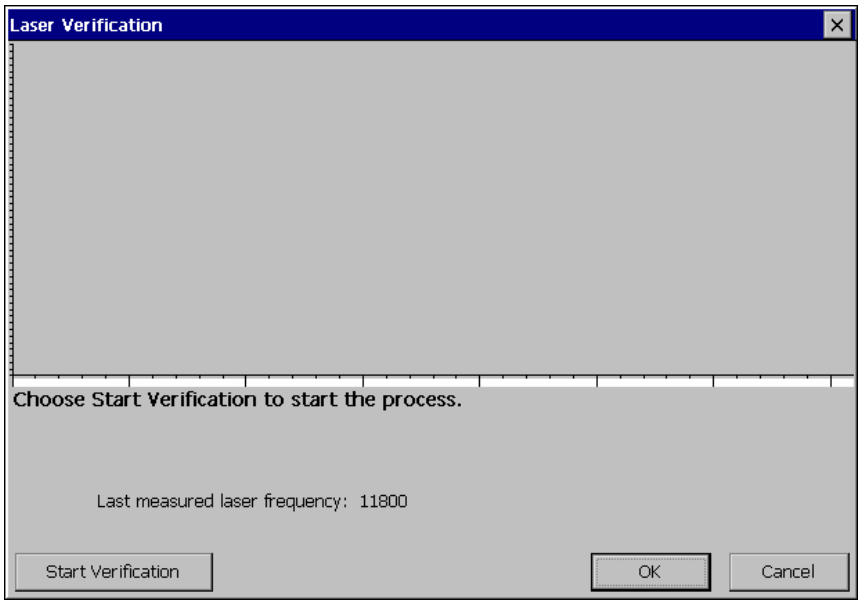
Note For optimum performance we recommend periodically verifying the laser on a Nicolet IR100 (that is not part of a Transport Kit) or Nicolet IR200. The software will prompt you when it is time to perform a verification. ▲

When you click the button, a message asks you to clear the sample compartment and turn off the purge if the system is purged:



Remove all accessories and samples from the sample compartment, turn off the purge (if present) and then choose OK.

The Laser Verification window appears:



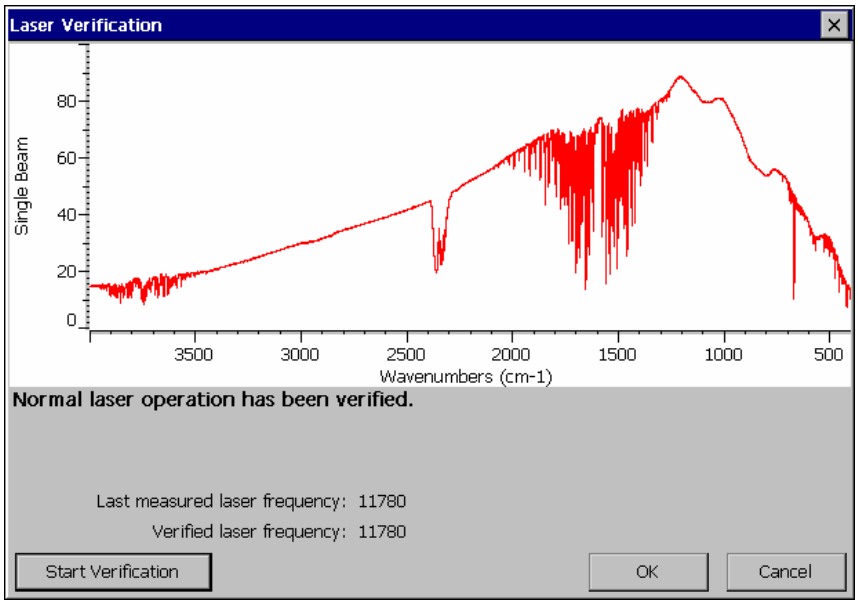
The window shows the last measured laser frequency.

Choose Start Verification to begin the laser verification (on a Nicolet IR100 or Nicolet IR200) or laser amplitude adjustment (on a Transport Kit).

When the process is finished, the newly measured laser frequency appears below the previously measured frequency (see the following illustration). If you have a Transport Kit, choose OK and skip the rest of this step; the laser amplitude has been adjusted. (You can verify this by using the Show Status button as explained in step 2.)

A background spectrum collected during the verification appears at the top of the window.

If you have a Transport Kit, the background spectrum and verified laser frequency value do not appear.



In this example, the laser frequency has not changed. You can choose OK or Cancel to close the window.

If a significant change has occurred, text in the window informs you. Choose OK to use the new value, or choose Cancel if you want to continue using the old value. (The spectral quality of your collected spectra may be compromised if you decide to use the old value.)

4. **When you are finished using the Diagnostics window, choose Close.**

   If you turned off the purge in step 3, turn it back on before collecting data.

Troubleshooting

The table below describes some software and applications problems that could occur while you are using your spectrometer and explains how to solve them. After the table is a list of hardware problems that could occur. See the "Troubleshooting" chapter of the manual titled *Servicing Your Spectrometer* for more information on solving those problems.

Also see the "Diagnostics" chapter, which explains how to use the Diagnostics command available through the Collect button to check the operation of the laser, source and moving mirror.

If you are unable to solve a problem after following the provided instructions, contact Technical Support.

Problem	**Possible Cause**	**Solution**
You cannot add a spectrum to a user library.	The resolution of the spectrum is different from that of the library.	Collect the spectrum again at the same resolution as the library (first set Resolution in the Collect Options dialog box), and then add it to the library. See "Setting the resolution" in the "Software Management" chapter.
A spectrum has totally absorbing peaks.	A sample in a transmission experiment is too thick.	Use a thinner sample.

Problem	Possible Cause	Solution
Water peaks interfere with sample peaks of interest.	The background is old (does not represent current conditions).	Collect a new background. See “Collecting a background” in the “Collecting Spectra” chapter.
	The desiccant is no longer effective.	Check the desiccant and replace or dry it if needed. See “Checking the desiccant” in the “More About Your Spectrometer” chapter.
	The spectrometer is not purged.	You can reduce the water vapor inside the spectrometer by purging it. See the manual titled *Installing Your Spectrometer* for information on connecting the purge hardware.
	The spectrometer is not adequately purged.	Make sure the purge gas is correct and the purge flow rate is adequate. Allow the system three to five minutes to reestablish purge before collecting the spectrum.
Carbon dioxide peaks interfere with sample peaks of interest.	The background is old (does not reflect current conditions).	Collect a new background. See “Collecting a background” in the “Collecting Spectra” chapter.
	The spectrometer is not purged.	You can reduce the carbon dioxide inside the spectrometer by purging it. See the manual titled *Installing Your Spectrometer* for information on connecting the purge hardware.
	The spectrometer is not adequately purged.	Make sure the purge gas is correct and the purge flow rate is adequate. Allow the system three to five minutes to reestablish purge before collecting the spectrum.

Problem	Possible Cause	Solution
A spectrum contains fringes or channeling.	The sample has parallel, highly reflective sides that cause the infrared beam to bounce within the sample when it is placed perpendicular to the beam.	Create a new film using a matte press. Roughen the film slightly with silicon carbide paper or other suitable abrasive.
There are no peaks in a spectrum.	There is no sample in the infrared beam path.	Check the sample compartment or accessory to make sure the sample is properly positioned in the beam path.
	The Y scale of the spectral display is not optimized.	Click the View button and choose Full Display to expand the peaks.
	The sample was in the sample compartment when the background was collected.	Collect the background again, making sure the sample compartment is empty. Then collect the sample spectrum again.
	An accessory is not operating properly.	Use a reference sample (for example, polystyrene for a Transmission accessory) to verify the accessory operation. If the accessory is working properly, the sample may not have significant infrared absorption (see the next item).
	The sample is not “infrared-active” (for example, it may be an inorganic material or it may have an extremely low concentration).	Use a sample that exhibits significant mid-infrared absorption.
	A sample film in an attenuated total reflection (ATR) experiment is being held against the ATR crystal with uneven pressure or has poor contact with the crystal.	Make sure the sample is held evenly and has good contact with the crystal.

Problem	Possible Cause	Solution
A spectrum is too noisy.	The detector is saturated.	Reduce the gain setting. See “Setting the signal gain” in the “Software Management” chapter.
	The spectrometer is not properly aligned.	Align the spectrometer. See “Aligning the beamsplitter” in the “Servicing Your Spectrometer” chapter of the manual titled *Servicing Your Spectrometer*.
	There were too few scans.	Increase the number of scans. See “Setting the number of scans” in the “Software Management” chapter.
	The resolution was too high.	Reduce the resolution (use a larger numerical setting). See “Setting the resolution” in the “Software Management” chapter.
The baseline of a spectrum is not flat.	A KBr pellet was made with coarsely ground KBr powder, or the KBr pellet was improperly pressed.	Be sure to press the pellet properly.
	The spectrometer is not properly aligned, causing a sloped baseline.	Align the spectrometer. See “Aligning the beamsplitter” in the “Servicing Your Spectrometer” chapter of the manual titled *Servicing Your Spectrometer*.
	Spectrometer has not been on long enough to reach thermal equilibrium.	For best results allow spectrometer at least one hour to stabilize after turning it on.
	The spectrometer is not properly purged.	Check the system to make sure correct the purge gas is being used and that the flow rate is correct.

Problem	Possible Cause	Solution
The interferogram peak in the Diagnostics window is flattened ("clipped").	The gain is set too high.	Reduce the gain setting until the signal intensity with no sample or accessory installed is between 7.5 and 8.5 volts. (Use the absolute value of the larger of the Peak Maximum and Peak Minimum values in the Diagnostics window.) See "Setting the signal gain" in the "Software Management" chapter.
No interferogram appears in the Diagnostics window, or the signal intensity is very low.	The infrared beam is blocked.	Remove any obstruction from the beam path within the sample compartment or under the spectrometer cover. For instructions for removing the cover and an illustration showing the normal position of internal components, see "Removing the main cover" and "Spectrometer components" in the "Servicing Your Spectrometer" chapter of the manual titled *Servicing Your Spectrometer*. Follow all safety precautions given in the manual. **Warning:** Turn off the spectrometer power and disconnect the power cord before opening the cover.
	An accessory is installed incorrectly.	Remove and reinstall the accessory. Follow the instructions in the manual provided with the accessory.
	The sample is highly absorbing.	Use a thinner sample.

Problem	Possible Cause	Solution
The results of a spectral subtraction or library search are incorrect, or the X-axis positions of peaks in a spectrum are incorrect.	The laser needs to be verified.	Use the Laser Verification button in the Diagnostics window, available through the Collect button. See the procedure in the "Diagnostics" chapter for details.
A data collection stops before it is finished (the gauge showing the progress of the collection stops changing), or there is a flat line or no interferogram at all in the live display of the Diagnostics window.	A major change in the ambient temperature has occurred.	If you are collecting a spectrum, choose Cancel in the dialog box containing the collection progress gauge to end the collection procedure. Allow time for the system temperature to equilibrate before collecting spectra. (Make sure the ambient temperature is within the allowed range.) The interferogram should be displayed normally in the Diagnostics window once the system is equilibrated.
	Environmental vibration is affecting the performance of the spectrometer.	Eliminate the source of vibration (for example, turn off nearby equipment) or place the spectrometer in a vibration isolation system.

The following symptoms can be caused by hardware problems. For information on solving these problems, see the "Troubleshooting" chapter of the manual titled *Servicing Your Spectrometer*.

- The Power item in the Diagnostics window shows an X (test failure).
- The Laser item in the Diagnostics window shows an X (test failure).
- The Source item in the Diagnostics window shows an X (test failure).
- The Moving Mirror item in the Diagnostics window shows a red X (test failure).

- The power indicator or power supply indicator is not lit.
- The built-in display on a Nicolet IR100 is dark.
- The humidity indicator has turned pink or white.
- The live display in the Diagnostics window shows a flat line or a very small signal.
- The live display in the Diagnostics window shows no signal at all.
- A message in the spectral display says the interferogram peak cannot be found.
- The interferogram peak in the Diagnostics window is not centered.
- Sample spectra show noise in the range from 4,000 to 3,000 wavenumbers.
- Sample spectra show noise across the spectrum.
- Sample spectra show large noise spikes.
- Ratioed spectra show significant baseline drift.
- The software informs you that the instrument is not scanning.
- Sample spectra have poor quality.

Index

d

e

f

g

n

o

p

t

u

v

w

x

y

z