MN-FTI-A170-E

FTI-A170
FOURIER TRANSFORM INFRARED SPECTROMETER
OPERATION MANUAL

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OF THE PRODUCTS.

VIDEO

INSIZE

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1 SAFETY AND GENERAL INFORMATION

This operator's manual contains information needed to install, operate the instrument and perform user maintenance.

This spectrometer is supposed to be operated by qualified personnel.

1.1 Fire Safety and Burn Hazards

To avoid a burn injury and the risk of fire or explosion, follow these guidelines:

Do not test flammable or explosive samples.

Use nitrogen or dried air only to purge your spectrometer and accessories.

After you turn off your spectrometer, wait 15 minutes before you replace components.

Never block the vents on a spectrometer power supply or on the spectrometer itself.

Use exact replacements for power supplies, variations in power supply specifications affect the safety of your instrument.

Touching the laser poses no burn hazard. If you must replace the laser assembly, you can begin the procedure immediately after turning off the spectrometer power.

Do not use harsh detergents, solvents, chemicals or abrasives; these can damage the finish. To avoid damaging port windows, do not allow liquid to run down to these windows.

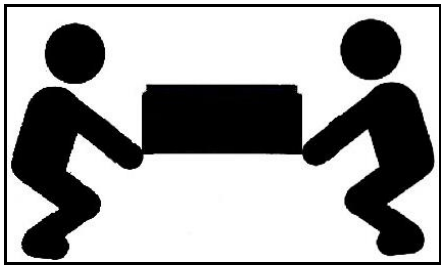
Do not attempt to clean or even touch the mirror surfaces. The mirrors in your spectrometer are front surfaced and can be easily scratched. Dust will not harm the infrared signal, but fingerprints can degrade spectral performance or permanently damage the mirrors. If you feel it is necessary, remove dust with a gentle stream of clean air or nitrogen. Use purge air only for cleaning mirrors; commercially prepared canned air contains contaminants that can damage the mirror surface or interfere with spectral data.

1.2 Lifting or Moving the Spectrometer

To avoid risk of injury, always use proper lifting techniques when lifting or moving the spectrometer or other system components.

Please keep strong shock away from the spectrometer while moving the spectrometer.

If you have attached a large accessory (such as a microscope) to your spectrometer, it must be removed before you attempt to lift or move the spectrometer.



1.3 Electrical Safety

Your spectrometer, computer, and accessories were designed with protective covers to prevent exposure to dangerous voltage and other electrical hazards. If you see either of the following symbols on your spectrometer or power supply, there is a risk of electric shock in the vicinity of the symbol.

If a protective cover on the spectrometer, power supply, or computer appears damaged, turn off the system and secure it against any unintended operation. Contact manufactory for service.

Even after the spectrometer has been disconnected from all voltage sources, capacitors may remain charged for up to 30 seconds.

You may also see one or more symbols on or near switches and connectors on your spectrometer. These symbols are often used to identify connectors or help you to locate user-replaceable fuses.

Alternating current

Direct current

Earth terminal or ground

Protective conductor terminal

Fuse

Power on

Power off

Caution, refer to the accompanying documents

Power Source

To turn on an IR Series spectrometer, press the power switch.

Do not turn on the power to your spectrometer until all other devices, like a printer or a computer, have been connected.

To avoid injury, only a qualified person using the appropriate measuring device should check the line voltage, current and frequency.

Be sure the power switch is in the off (O) position before you connect the power supply to your spectrometer.
1. Connect the DC power cable to the spectrometer.
2. Connect the AC power cable to the external power supply.
3. Connect the AC power cable to AC power source.

Fuse

The IR Series spectrometers are protected by two, 2A. The fuses for these spectrometers are not individually replaceable.

Ground Wire

Each wall outlet you use must be equipped with a 3-wire line: live, neutral, and ground. The ground must be a non-current carrying wire connected to earth ground at the main distribution box. To assure a good ground connection and avoid shock hazard, do not use an outlet that has ground connected to a conduit ground.

Do not disconnect protective earth terminals inside the spectrometer when the power is on. Doing so would create a shock hazard.

You must be sure to use an appropriate power cord for the electrical service. The power cord supplied with the spectrometer is a 3-wire, grounded power cord, appropriate for use in the country listed as the shipping destination for the spectrometer. If the power cord you received is not appropriate for the electrical system in your location, contact TianJin GangDong Sci & Tech. Development Co. Ltd Customer Support and order a new power cord.

To prevent electrical hazards, do not remove or defeat the ground prong on the power cord. If you use an extension cord, it also must have a protective conductor.

1.4 Laser Safety

IR Series spectrometers are laser products.

Never stare into the laser beam or at its reflection. Never tamper with the laser head, even if you are replacing a defective laser. Exposure to laser light or high voltage may result.

For your saftey, please be sure the power is cut off before the moving

protective cover of the spectrometer.

To protect your eyes

Exposure to invisible radiation from the diode laser can result in serious injury and/or blindness. To avoid serious injury, wear laser safety goggles whenever the power must be turned on after the interferometer cover has been removed from an spectrometer.

Always verify that the wavelength(s) listed on your eye wear correspond to the wavelength(s) of the laser being used.

Using laser goggles

Whenever you use laser safety goggles, follow these guidelines.

Check your goggles before use for pits, cracks, flaws, scratches, discoloration or other damage. If you find any type of damage, replace the eye wear immediately.

Avoid direct exposure to chemical vapors or chemical liquids that could cause surface cracks or other damage.

Check your goggles before use to assure that the wavelength(s) listed on the eye wear matches the wavelength(s) of the laser being used.

Make sure that the goggles fit securely. If they do not fit properly, they cannot provide protection from laser radiation.

Never use laser safety goggles:

for viewing direct beams or specular reflections
during recreational or sports activities
as sunglasses
while operating a motor vehicle
as protection against high impact or hazardous chemicals, or during welding, brazing, or cutting operations.

Use only mild soap and water to clean your goggles. Ammonia, alkaline cleaners, abrasives and solvents can damage the lenses.

1.5 Caustic or Corrsive Agents

Spectrometer components may be degraded by exposure to caustic or corrosive agents or their vapors. To maintain the spectrometer in safe working condition, do not use caustic agents. Damage to the spectrometer caused by the use of caustic agents is not covered by the warranty.

Chlorinated solvents, perfluorochlorinated solvents, and other solvents containing halogenated hydrocarbons are often used as sample solvents. The pyrolysis of these solvents by an infrared source or by

excessive heating caused by laser absorption may produce hydrochloric acid (HCl), hydrofluoric acid (HF), or phosgene (COCl).

Hydrochloric acid and hydrofluoric acid are highly corrosive and may cause accelerated corrosion of the metallic components in the spectrometer. Damage may be caused in any spectrometer, if the concentration level of corrosive gases in the air is excessively high due to improper sampling techniques.

2 INSTALLATION

2.1 Unpacking and Inspection

Prior to opening the shipping container, inspect it for damage or evidence of mishandling. If it has been damaged or mishandled, notify the carrier before opening the container. Once the container is opened, inspect the contents for damage. Any damage should be reported to the carrier immediately. Save the shipping container. Check the contents against the packing list.

To avoid irreparable damage to your spectrometer, open the shipping box, but not the plastic bag around the spectrometer, in the room where the instrument will be used. Wait 24 hours before removing the plastic bag. This allows your spectrometer to come to room temperature and protects delicate optical components.

2.2 Location/Environment

The preferred environment for the spectrometer pump is normal laboratory conditions. The area should be clean and have a stable temperature (16℃~25℃,60℉~78℉) and humidity (20%~60%). The instrument should be located on a stable flat surface with surrounding space for ventilation and the necessary electrical and fluid connections.

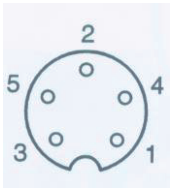
Risk of affected with damp is one of the most worries. Spectrometer contains a container of desiccant that keeps the optics compartment free of water vapor. This protects the beam splitter and other optical components from moisture damage. However, we still recommended you to keep your lab dry.

2.3 Connection

To install and operate the spectrometer, please follow the instructions in the manual when installing your spectrometer. This will help you to get reliable spectra with safely.
This spectrometer is supposed to be operated by trained personnel.

Power
Power Switch is at the rear panel of the spectrometer
O = off
I = on

Do not turn on the power to your spectrometer until all other devices, like a printer or a computer, have been connected.



Power Supply
A special power supply is supplied with the spectrometer.

1 COMMON SHELL:GND
2 COMMON SHELL:GND
3 5V
4 COMMON SHELL:GND
5 12V

To avoid injury, only a qualified person using the appropriate measuring device should check the line voltage, current and frequency.

Connect your spectrometer with the power supply.

3 TURNING ON THE SPECTROMETER

3.1 Warm up the Spectrometer

1.To turn on an IR Series spectrometer, press the power switch.

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.

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

2.Turn on your PC and strart the FTIR application. Check if the pc can communicate with your spectrometer.

3.Every time before using this spectrometer, wavelength has to be checked and calibrated. If the spectrometer does not work in order, please check and troubleshoot before collecting spectra.
Click on Experiment Setup under Acquisition and select Diagnosis. If a  appears, which shows something wrong with the spectrometer. When trouble is removed. Select “Optical Bench” and check gain. Adjust gain if it is not within acceptable range.

4.Now you can make measurement and collect spectra.

3.2 Measurement Procedure

1 Sample preparation

Before sample preparation, KBr must be test to see if it meets requirements. Make KBr as blank slice and tested in spectrometer with air as reference sample.

Before every test, place some KBr in weighing bottle and put it under IR source for 1 hour or bake under 105℃ for 3 hours. Then put it in dryer for future use.

2 Casting KBr Crystle

Put 0.3 mg sample which residual moisture has been drive off (illuminated under IR source 1 hour or bake under 105℃ for 3 hours) in agate mortar and add some dry KBr made on previous step. Grind them in same direction until well mixed. Take mixed powder to die and to a tablet press with air pressure 10t/cm^2 for 3minutes.

Take the sample card off from the tablet press, check if it is even, surface of good quality, and light can go through.

3. Collecting Background

Click Collect/ Collect Background. A collect background prompt is displayed. Take sample out from the sample compartment and insert blank card, then Click OK.

4 Scan Sample

Click Collect/ Collect Sample. A scan sample prompt is displayed. Take Blank sheet out from the sample compartment and insert sample. Click OK.

5. When sample scanning is finished, the application will extract background from data collected and displays spectrum of sample scanned.

6. Process spectra collected.

3.3 Finishing Measurement

1. Exit FTIR application.
2. Turn off the spectrometer.
3. Remove sample in sample compartment.
4. Clean the spectrometer and other tools.
5. Turing off your PC.
6. Make measurement report.

Plug off the cable from wall socket if necessary.

4 SERVICE AND MAINTENANCE

Your IR Series spectrometer can operate reliably under adverse conditions, but to obtain the best performance possible, there are some routine maintenance and service procedures you should perform. This manual contains instructions for replacing, servicing, and maintaining the components of your spectrometer and complete information about these procedures and is divided into the following chapters:

- Cleaning Your Spectrometer
- Gain Adjustment
- Changing Desiccant Canister
- Changing Laser
- Changing IR Source
- Changing Windows

Most of these services are supposed to be performed when very necessary. However, changing and reuse desiccant must be done regularly.

Before servicing the spectrometer, please plug off the cable and there is no hazard of laser radiation and high voltage.

Static electricity

Static electricity can permanently damage the electronics in your spectrometer, so you should always discharge any static electricity build up in your body before

opening the main cover of your spectrometer

touching power supply, light source, electronics, metal part of the spectrometer.

4.1 Cleaning Your Spectrometer

Never use a flammable gas to purge a spectrometer. The purge gas must be free of oil and other reactive materials. Heat from the source or from laser absorption may ignite flammable gases or reactive materials in purge gas.

If the outside of the spectrometer needs cleaning, turn off the power and disconnect the power cord. Then use a damp (not wet), soft cloth and a mild soap to clean the outside of the spectrometer. Do not use harsh detergents, solvents, chemicals or abrasives; these can damage the finish.

Avoid shock hazard. Do not allow liquid to run into the power supply. Also, do not allow liquids to run down the windows in the sample compartment chamber.

Cleaning the mold.

After making sample sheet, swap the mold with soft tissue and wash residue sample with solvents until no sample could be seen by naked eye. Then flash with distilled water for three times and dry the mold under IR light for one hour. Keep the mold in container free from dump.

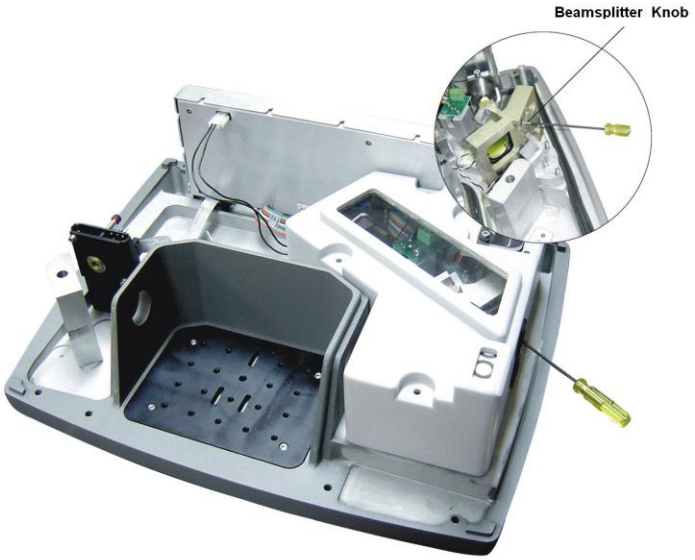
Clean the spectrometer

Keep the spectrometer free from sample powder. Check if Silica Gel in sample compartment is dry and no residue samples of previous test. When test is done, take samples out of the compartment. Wipe the compartment and surface of the spectrometer with soft tissue until no powder or liquid left.

4.2 Gain Adjustment

Click Collect/Collection Setting/Bench and use a screw driver to turn knob of beamsplitter while check if the gain in Optical Bench within acceptable range.

Please turn the knob slowly and carefully.



4.3 Changing Desiccant Canister

The desiccant canister holds a material that absorbs moisture inside your spectrometer. When this material becomes saturated, the humidity indicator turns pink or white, and the desiccant canister must be dried out or replaced with a new canister.

If the spectrometer is not supposed to use for a relativly long period, please change desiccant every two weeks. Please turn on the spectrometer every week for at least 4 hours.

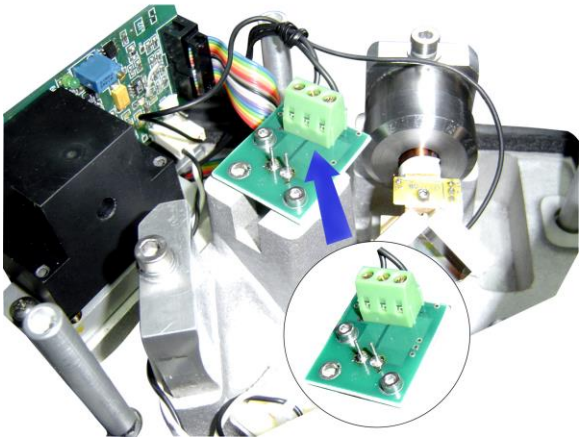
You will need a vented oven and an insulated cloth or hot pad. If you are going to dry and reuse a saturated desiccant canister, make sure you have a fresh desiccant canister you can place in your spectrometer while the saturated canister dries.

Place the saturated desiccant canister in a vented oven at 150℃(about 300°F) for three hours.

Do not leave the canister in the oven for more than three hours and do not exceed a temperature of 150°C (about 300°F).

4.4 Changing IR Source

The source contains an element that is heated electrically to produce infrared radiation. Use the following procedure if you have to replace the source.



4.5 Changing Laser

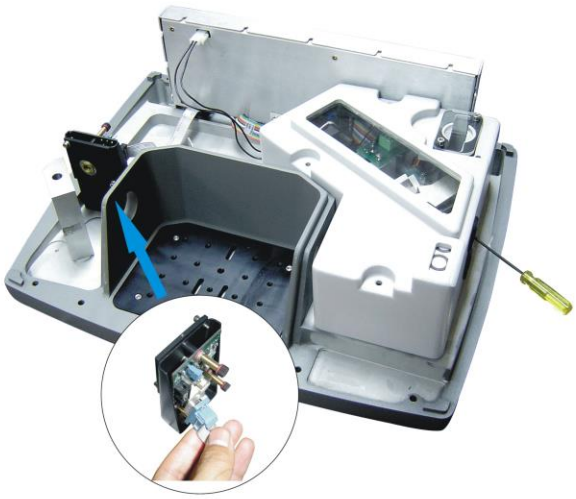
The laser provides the reference signal for triggering data collections and measuring the stroke of the moving mirror. The instructions below explain how to replace the diode laser.

To avoid exposure to invisible Class IIIb laser radiation, never stare into the diode laser, and always make sure the power is turned off and all cables are disconnected from your spectrometer while the interferometer cover is removed.

Turn off the spectrometer power, disconnect the power cable and all other cables from the back of your spectrometer, and then remove the main cover and the interferometer cover.

To avoid hazardous exposure to visible or invisible laser radiation, never stare into the diode laser or the bright red laser beam (or a reflection of the beam) emitted by the He-Ne laser, and always make sure the power is turned off and all cables are disconnected from your spectrometer while the interferometer cover is removed.

Be sure to turn off the spectrometer power, disconnect the power cable and all other cables from the back of your spectrometer before changing IR source



4.6 Changing Window

The plastic cover that goes over the interferometer has a KBr window through which the infrared beam passes when it goes into the sample compartment. If this window becomes fogged by condensation, you will have to replace it using the following instructions. You will need a flat-blade screwdriver and clean gloves or finger cots.

KBr windows are very delicate and can be permanently damaged by skin oils or other deposits. When handling a KBr window, always wear clean gloves or finger cots.

5 Specifications

WN Range……	7800-350 cm^{-1}
WN Accuracy…… ...	1.0 cm^{-1}
Transmittance Repeatability……	± 0.5%
SNR……	30000:1(1min, 2100 cm^{-1})
100% Line Flatness and Straightness	99%-101%(4000 cm^{-1} ~500 cm^{-1})
Power Source……	AC 100V~240V, 47~63 Hz
Dimensions……	Mainframe: 450mm× 350mm ×205mm
Weight……	14kg or so

Software Manual

1. Introduction

The software is a Windows-based software application is used to control the spectrometer, manage, process and extract information from spectra collected.

2. Installation

2.1 Minimum PC Requirements

To ensure a successful installation of the software, please check blow requirements before starting the installation:

- Intel Pentium processor with 500 MHz or greater.
- At least 128 MB RAM
- The capability of displaying high color (6bit) at 1024X768SVGA
- Quad speed CD-ROM drive
- Hard disc with at least 1G free space
- A keyboard, printer and mouse
- USB 2.0 interface
- One of the following operating systems
  Windows 98 with Internet Explorer 5.0 or later.
  Windows XP or later

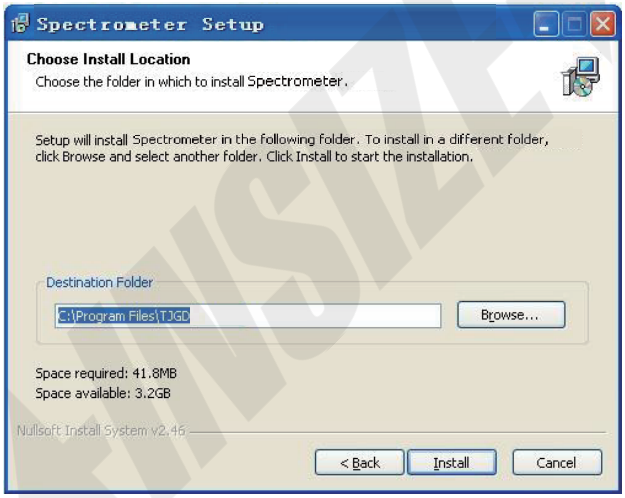
2.2 Installing the Software

The application has a Wizard to help you install the software on your PC

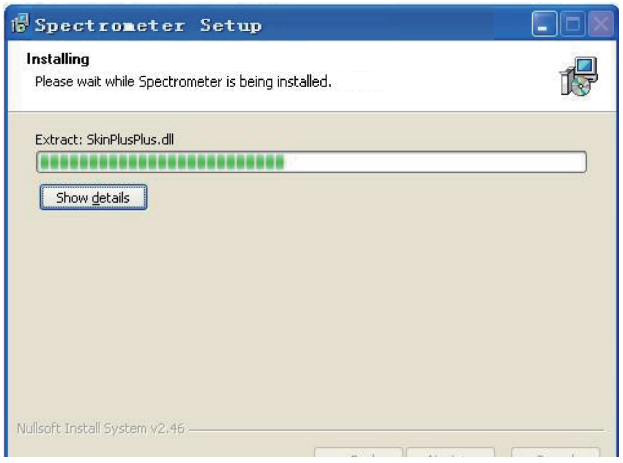
1. Set up and connect the spectrometer and PC as discussed in the user manual. Place the software CD into CD drive. Browse CD and double click on FTI-A170 x.x.x Setup.exe to run the installer software. And then you can select Installer language as followed picture shown.

You can select Chinese(Simplefied) or English,If you run this software on an English OS,this picture would not be shown and English will be selected as default. Now click the OK button.

2. Click Next to continue or Cancel to exit setup.



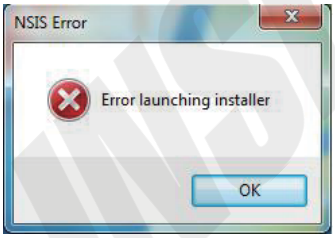
3. Specify a location path and click Install.



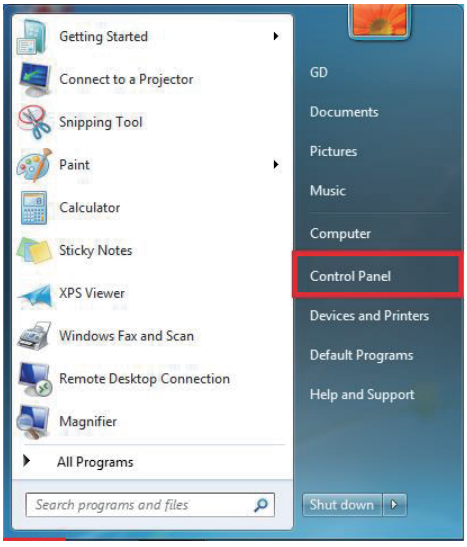
4. Click Finish to close the installer.

2.2.1 Installation FAQ

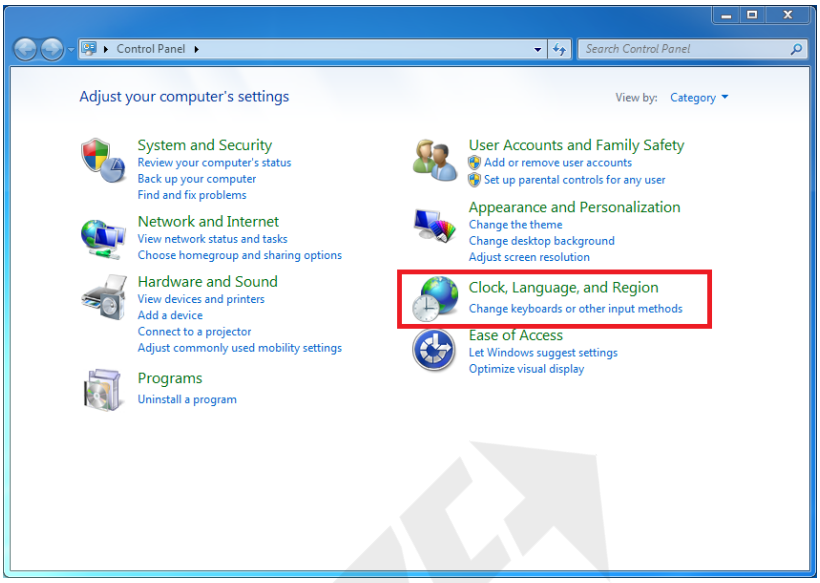
Prompt "Error Launching installer" when installing the software.



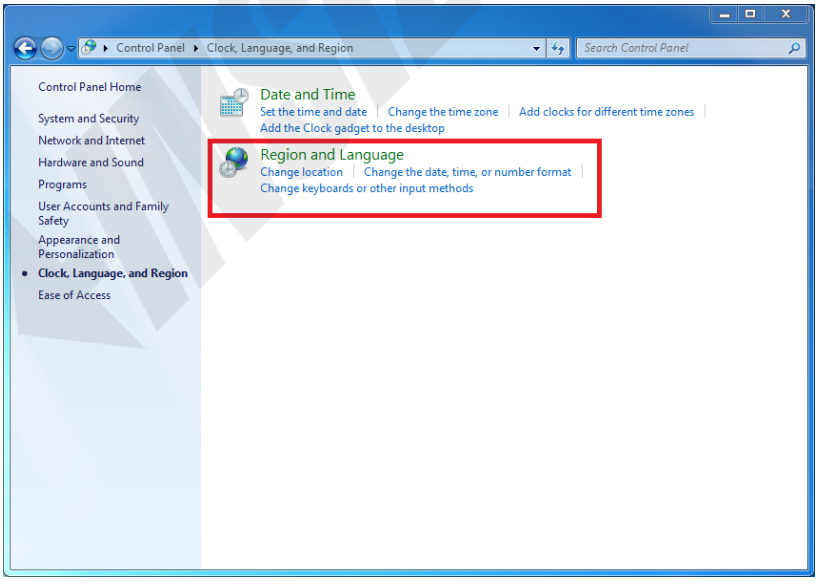
1. Click on "Start" menu and then click on "Control Panel"



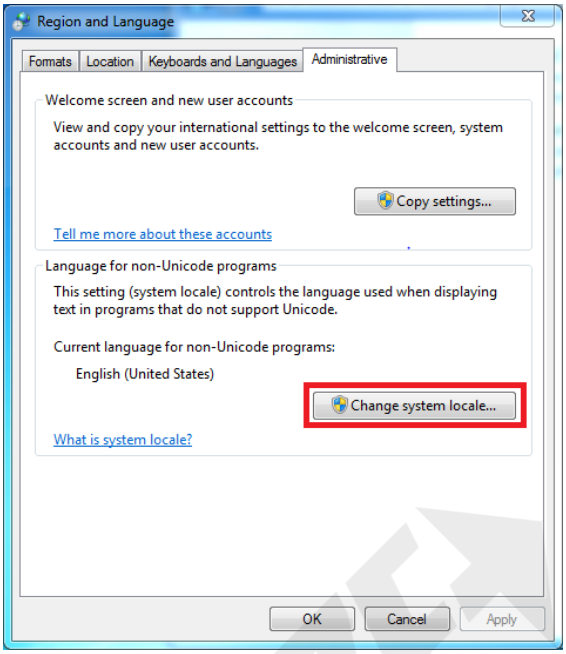
2. Click on “Clock, Language, and Region”.



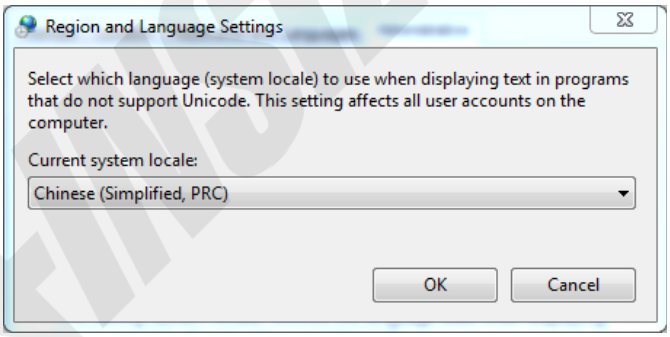
3. Click on “Region and Language”.



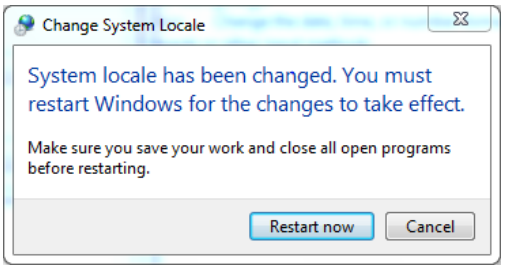
4. Select the “Administrative” and then click on “Change system locale…”.



5. Select “Chinese (Simplified, PRC)” and then click on “OK”.



6. Click on “Restart now” and then install the software again after restarting.



2.3 Install the USB Driver

Before using the software, USB driver has to be installed:

1. Place the CD supplied into CD drive
2. Connect the PC and FTIR spectrometer with a USB cable.
3. Power on FTIR spectrometer, an installation wizard is displayed.
4. Select application path, “X:\USB-DRIVER”,click Next until finished.

If the system can not find the CD or file, reselect the application path.

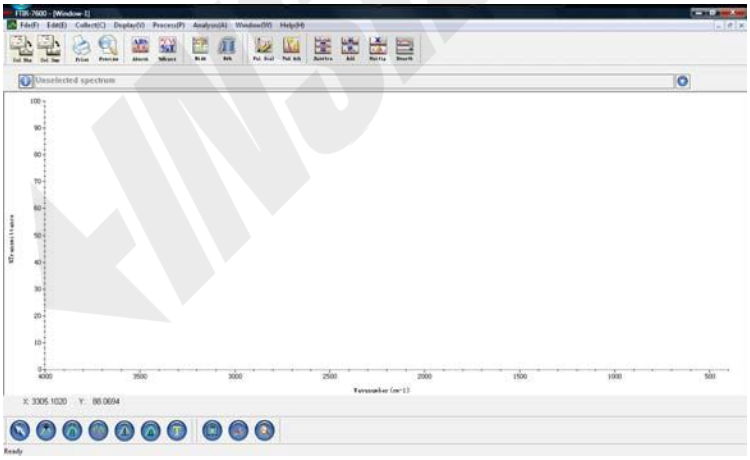
Once the software and USB driver installation is complete, the instrument is ready to use.

3. Operate the Software

Switch on the spectrometer as detailed in the user manual.

1. Turn on the PC.
2. From the windows start menu, select ‘FTI-A170 Spectrometer’ under ‘All Programs’ or you can click on the desktop shortcut.

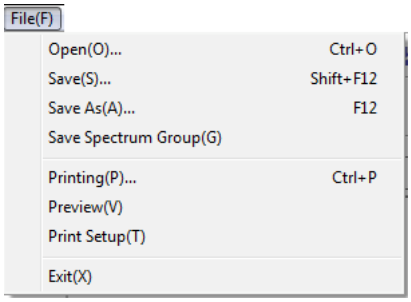
The software starts and a main interface window is displayed.



4. Software Functions

4.1 File

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



To do this...	**Use command**...
Retrieve spectra saved on a disk.	Open
Save a spectrum on a disk.	Save
Save a spectrum using a new file name	Save As
Save a group of spectra.	Save Spectrum Group
Print or plot the results of your work.	Printing
Preview the file before print.	Preview
Set up the system printer.	Printer Setup
Exit FTIR.	Exit

4.1.1 Open

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

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

Opening a CSV text file

CSV (comma-separated values) text files contain data in the form of pairs of X and Y values. If you save a spectrum as a CSV file, you can process the data using a spreadsheet program. You can use FTIR to open and display a CSV text file as a spectrum and save it into spectral data file with the axis units you specify.

The CSV file should meet the following requirements to be opened.

It is a text file (with the extension .CSV) consisting of a list of pairs of X and Y values.

Each pair is on a separate line and each line is ended by pressing the Return or Enter key.

There is a comma tab, space or line feed between the X and Y values.

The X values are in increasing order.

Opening a spectrum by choosing its filename from the File menu

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

1. Select Open from the File menu.

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

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

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

3. Select OK.

If you are opening a CSV text file, the parameters dialog box lets you set several parameters that affect the conversion of the data or that record information about the spectrum.
If the file you are opening contains evenly spaced data points, you can use the default settings. If the file contains unevenly spaced data points, set the appropriate parameters.

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

Depending on the software option settings and whether a spectral window is opened, the spectra opened may appear in the active spectral window or in a new window. The spectrum

that is opened last is selected and can immediately be used in other operations.

4.1.2 Save

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

1. Select the spectrum.

If not already selected use the drop down menu to select.

2. Select Save from the File menu.

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

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

You can specify a default directory for this operation in the File options (available through Options in the Edit menu).

4. Select OK.

4.1.3 Save As

Use Save As in the File menu to save one or more spectra in files on a disk using new file names.

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

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

Save spectra using new file names

1. Select the spectra.

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

2. Choose Save As from the File menu.

The Save As dialog box appears.

3. Type a file name for the first spectrum in the File Name text box.

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

You can specify a default directory in the File options (available through Options in the Edit menu).

5. Select Save.

If there are no more selected spectra to save, the procedure is finished.

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

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

4.1.4 Save Spectrum Group

Use Save Spectrum Group in the File menu to save multiple spectra as a group with the file extension .SPG. You can open the group later by using Open in the File menu.

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

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

2. Select 'Save Spectrum Group' from the File menu.

The Save Group dialog box appears. This is a standard Windows dialog box.

3. Type a file name for the group.

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

You can specify a default directory in the File options.

5. Select Save.

4.1.5 Printing

Use Print in the File menu to print spectra in a spectral Window. When you print spectra contained in a spectral window, they are printed in the same order as they appear on the screen. If you are displaying a spectral region, that region is printed.

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

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

The changes you make to the Print options will take effect when you print a spectral window (or a report using Preview/Print Report). The display of spectra in a spectral window is not affected by the Print options.

2. Display the items you want to print.

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

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

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

4. Select Print from the File menu.

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

4.1.6 Preview

Use Preview in the File menu to preview the spectra before printing. Printing can also been done in this function by clicking the print button.

4.1.7 Print Setup

1. Select Print Setup from the File menu.

The Print Setup dialog box appears.

2. Select the printer from the list box.

You can also specify portrait or landscape page orientation. If you change the orientation using Printer Setup, the Orientation option in the Print options (available through Options in the Edit menu) will be reset to the new orientation. The page orientation setting in Windows Control Panel or in the printer setup dialog box for other applications is not affected by the setting you make here.

3. If you want to set the printer parameters, select Options. If you don't want to set the parameters, select OK.

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

4.1.8 Exit

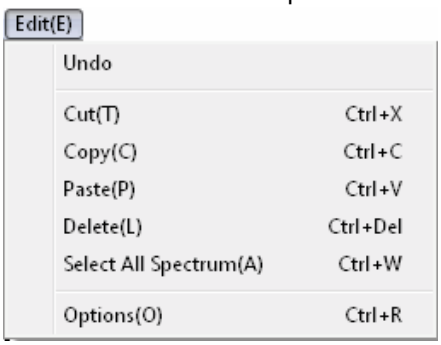
Use Exit in the File menu to Exit the application.

Select Exit from the File menu.

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

4.2 Edit

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



To do this...	**Use this command**...
Revert item in a window.	Undo
Remove item from a window.	Cut
Copy item in a window.	Copy
Paste item into a window.	Paste
Delete spectra from a spectral window.	Delete
Select all the spectra in a spectral window.	Select All Spectrum
Customize the software by setting options that affect its operation.	Options

4.2.1 Undo

Revert item in a window which is deleted by last time.

4.2.2 Cut

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

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

1. Select the items.

To select a spectra use the drop down list.

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

2. Choose Cut from the Edit menu.

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

4.2.3 Copy

spectra, text or images onto the Windows Clipboard (replacing the previous contents, if any). After you copy an item, you can use Paste to paste a copy of the item into another location. (The location can be in FTIR or in another appropriate Windows application such as a spreadsheet, word processing or graphics program.)

1. Select the items.

To select a spectra use the drop down list.

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

2. Choose Copy from the Edit menu.

The items are copied onto the Windows Clipboard.

4.2.4 Paste

After you cut or copy spectra, text, you can use Paste in the Edit menu to place a copy of the items in the location you specify.

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

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

1. Click the spectral window or location where you want to paste the items.

2. Select Paste from the Edit menu.

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

4.2.5 Delete

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

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

1. Select the spectra you want to clear.

2. Choose Delete from the Edit menu.

4.2.6 Select All Spectrum

1. Select the spectral window.

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

2. Choose Select All from the Edit menu.

All the spectra that are not hidden become selected.

4.2.7 Options

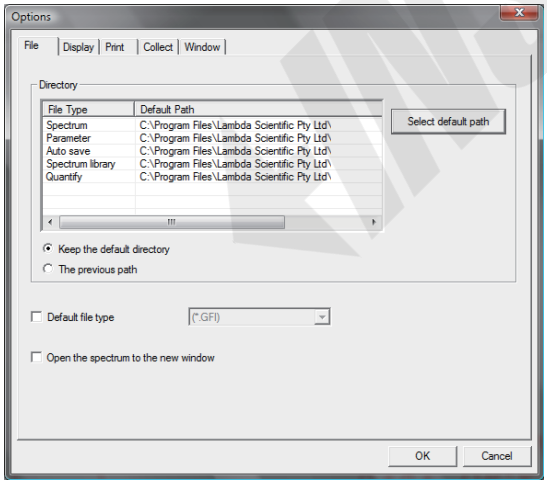
Use Options in the Edit menu to customize the FTIR-650 settings for the way you prefer to use the software. You can set options that affect how spectra are collected, displayed, processed, saved and printed.

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

The following sections describe the five sets of options.

4.2.7.1 File

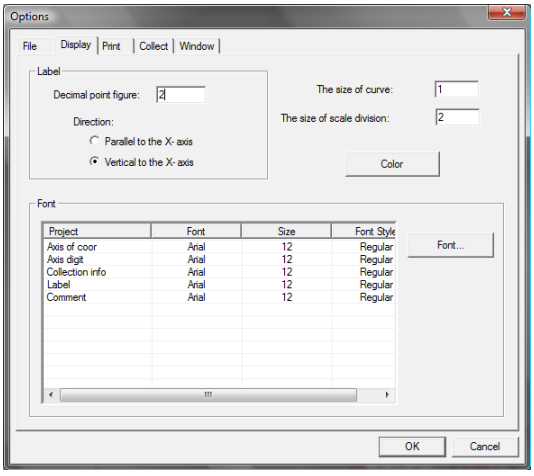
The File options appear when you click the File tab.



The following table shows what you can specify with the File options.

To specify or do this…	Use this feature…
The default directories for operations.	Directory
The default file format for opening and saving spectra	Default file type
Place opened spectra into new spectral windows	Open the spectrum to the new window

The Display options appear when you click the Display tab.

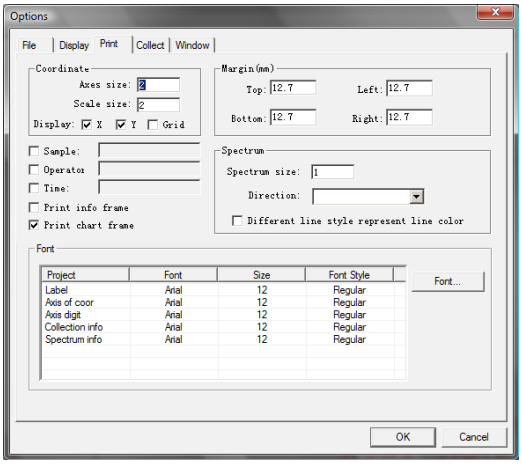


The Display options let you specify how to display items in spectral windows. The table below shows what you can specify with each option.

To specify this…	**Use this feature**…
The number of decimal places in annotations.	Decimal point
The orientation of annotation text.	Direction
The thickness of tick marks of displayed axes.	The size of curve
The line thickness for displaying spectra.	The size of scale division
The colors for displaying spectra and other features.	Color
The style of displayed text.	Font Style
The fonts for displaying text.	Fonts

4.2.7.3 Print

The Print options appear when you click the Print tab. The Print options affect how spectra and other images in spectral windows or in reports are printed on paper.

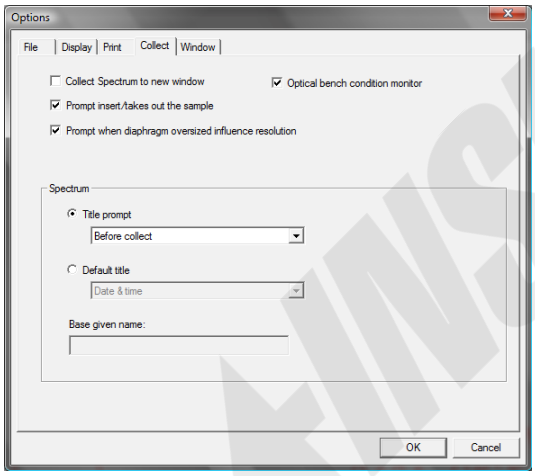


The table below shows what you can specify with each option.

To specify or do this…	Use this feature…
The thickness of printed axes.	Axes size
The thickness of printed axis tick marks.	Scale size
Print the X-axis.	X
Print the Y-axis.	Y
Print a grid with spectra.	Grid
Print the name of sample.	Sample
Print the name of operator.	Operator
Print the date and time.	Time
Print a box around spectra.	Print chart frame
The margins for printing.	Margins
The line thickness of printed spectra.	Line Thickness
Print colors as line patterns.	Different line style represent color
The orientation of printed pages.	Direction
The fonts for printing text.	Font

4.2.7.4 Collect

The Collect options appear when you click the Collect tab.



To specify or do this…	Use this feature…
Place collected spectra into new spectral windows.	Collect spectra to new window
Display prompts to insert and remove samples.	Prompt insert /take out the sample
Display a warning if the aperture is too large for the selected resolution.	Prompt when oversized influence resolution
How to title collected spectra.	Spectrum

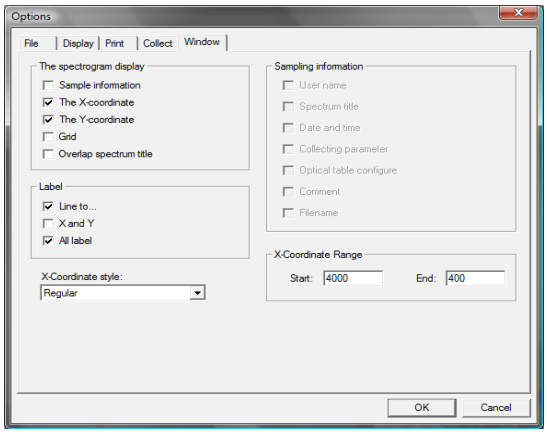
4.2.7.5 Window

The Window options affect the way spectra and other information will be displayed in new spectral windows. A new spectral window is created when you use New Window in the Window menu or use the window selection box to add a result spectrum from a task window to a new window.

The Window options settings serve as the defaults for new

spectral windows. You can change the way information is displayed in a window by using Display Setup in the Display menu or the Display options.

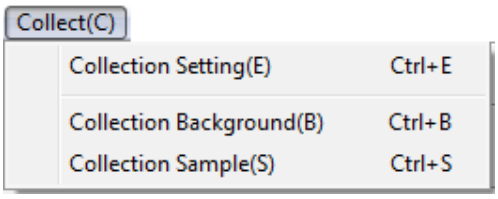
The table below shows what you can specify with each option.



To specify or do this...	**Use this feature**...
Display sampling information.	The spectrogram display
Display the X-axis.	The X-coordinate
Display the Y-axis.	The Y-coordinate
Display a grid with spectra.	Grid
Display overlaid spectrum titles.	Overlap spectrum titles
Connect annotation to spectra with a line.	Line to
Include both X and Y values in labels created with the annotation tool.	X and Y
The X-axis format for new spectral windows.	X-coordinate style
The sampling information to display.	Sampling Information
The X-axis display limits for new spectral windows.	X-coordinate range

4.3 Collect

The Collect menu includes commands for preparing the system for data collection and collecting spectra.



The table below summarizes the main use of each command:

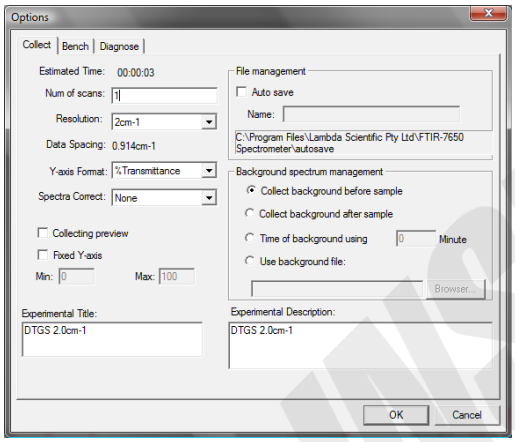
To do this...	**Use this command...**
Set the data collection parameters, perform diagnostic checks or align the spectrometer.	Collection Setting
Collect a background spectrum.	Collect Background
Collect a sample spectrum.	Collect Sample

4.3.1 Collection Setting

You can customize the way FTIR collects data by setting options using the Options command in the Edit menu. (see Options in the "Edit" chapter for details.)
Use Collection Setting in the Collect menu to set the parameters that control how spectra are collected—including which beam path and accessory are used—and how collected spectra are checked for quality. You can also use the command to perform diagnostic checks of the spectrometer and to align it.

After you set the parameters for a particular type of experiment, you can save the settings in a file named for that experiment type. When you want to perform a similar experiment later, you can quickly reset the parameters to the required settings by simply opening the appropriate experiment file.

4.3.1.1 Collect



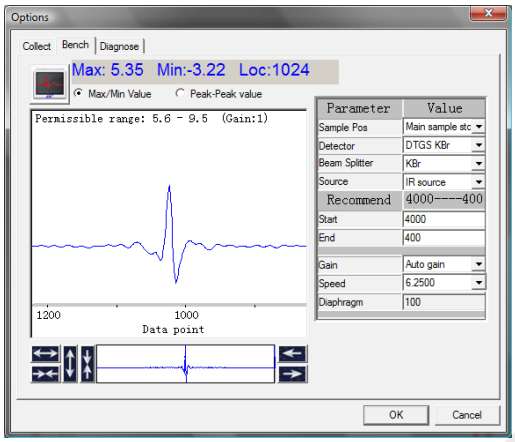
The Collect tab contains parameters for specifying the items shown and described in the following table.

To specify or do this…	**Set this parameter**…
The number of scans to collect.	Num of scans
The spectral resolution of the data.	Resolution
The Y-axis format of collected data.	Y-axis Format
The correction type to use.	Spectra Correct
Check the performance of the spectrometer at the start of data collection.	Collecting preview
The Y-axis display limits for the Collect Sample and Collect Background windows.	Fixed Y-Axis
The title of the experiment.	Experimental title
Save spectra automatically.	Auto Save
The base name for saving spectra automatically.	Name
Whether and when to collect a background spectrum or use a stored background, and how many background scans to collect.	Background spectrum management
A description of the experiment.	Experimental description

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

Setting	Y-Axis Format
Interference pattern	Interference pattern
Single beam	Single beam
% Transmittance	% Transmittance
Reflectance	% Reflectance.
Absorbance	Absorbance

4.3.1.2 Bench



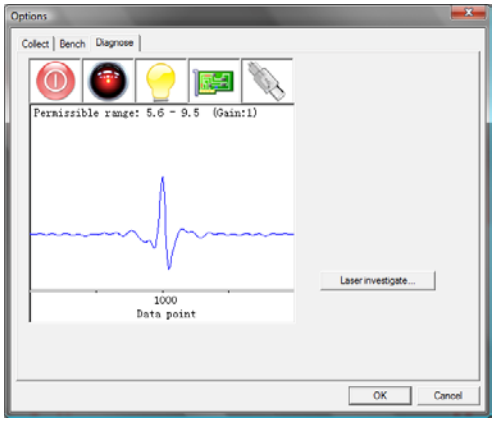
The Bench tab contains the parameters and other features shown and described in the following table.
At the left side of the Bench tab is a live display of the detector signal.

To specify or do this…	Use this feature…
Interact with the live display of the detector signal.	Live display
How to express the interferogram peak amplitude.	Min/Max value or Peak –Peak value
Display the signal as a single-beam spectrum.	Single Beam
The sample compartment to use.	Sample Pos
The detector type.	Detector
The beamsplitter type.	Beam Splitter
The source type.	Source
The spectral range to save.	Start/End
The detector signal gain.	Gain
The moving mirror velocity.	Speed
The aperture size.	Diaphragm

4.3.1.3 Diagnose

When you click the Diagnostic tab, special diagnostic and alignment features appear.

At the left side of the dialog box is a live display of the detector signal. This display is similar to the live display provided on the Bench tab.



Checking Spectrometer Components

You can check the operation of several spectrometer components. The components that correspond to the indicators are named below.


Power supply


He-Ne laser


Light source


Electronics


Beamsplitter and detector

When you click one of the first four indicators, a dialog box shows information about the status of the corresponding component. If this value is within the range shown in the acceptable range column, a check mark appears in the status column.

When you are finished viewing the information, select OK.

4.3.2 Collection Background

Use Collection Background in the Collect menu to collect a background spectrum. A background spectrum measures the response of the spectrometer without a sample in place. During collection a live display of the data appears.

A background spectrum is used to eliminate signals due to the spectrometer and its environment from the sample spectrum. The background single- beam spectrum shows how the energy of the source is distributed over the displayed frequency range.

4.3.3 Collection Sample

After you have selected an experiment, use Collection Sample in the Collect menu to collect the spectrum of a sample.

During collection a live display of the data appears in the Collect Sample window.

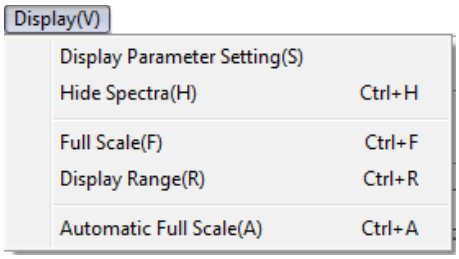
Viewing the progress of the collection

The progress of the collection is indicated visually by the gauge at the left side of the window just below the workspace. As data is collected, the gauge is gradually filled from left to right. For some spectrometers the number of scans collected so far and the total number of scans for the collection is displayed to the right of the

4.4 Display

You can customize the way FTIR displays spectra by setting options using the Options command in the Edit menu.

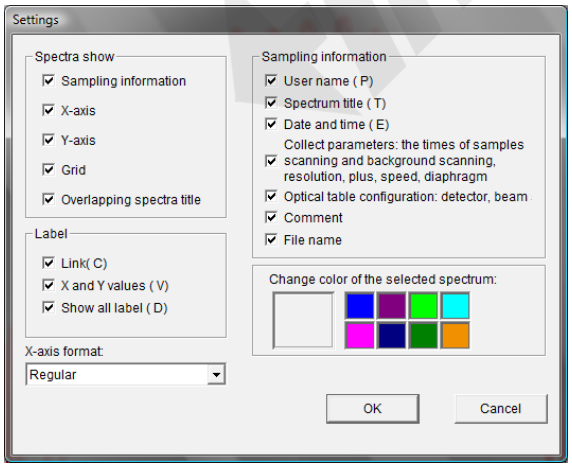
Use the commands in the Display menu to look at your spectral data in different ways. The primary use of each command is summarized in the following table:



To do this…	**Use this command**…
Set the display parameters for a spectral window.	Display Parameter Setting
Hide a spectrum from view.	Hide Spectra
Adjust the vertical scale of spectra so that they fit their panes.	Full Scale
Specify X-axis and Y-axis display limits for spectra.	Display Range
Display spectra full scale automatically after displaying a different spectral region.	Automatic Full Scale

4.4.1 Display Parameter Setting

Use Display Parameter Setting in the Display menu to specify how spectra are to be displayed in the currently active spectral window. The display parameters are provided in the Setting dialog box (see the following illustration).



If you create a new spectral window, it will use the Window options. The following table shows what you can specify with each parameter.

To specify or do this...	Set this parameter...
Display information about how a spectrum was collected.	Sampling Information
Display the X-axis.	X-Axis
Display the Y-axis.	Y-Axis
Display a grid indicating X and Y values.	Grid
Display the titles of all overlaid spectra.	Overlapping spectra titles
Connect annotations to spectra with a line.	Link
The X-axis format of spectral data.	X-axis Format
Display annotations for all spectra.	Show all labels
Include both the X and Y values in labels created with the annotation.	X and Y Values
The kinds of information included when sampling information is displayed.	Sampling Information
The color used to display spectra.	Change color of the selected spectrum

4.4.2 Hide Spectra

Use Hide Spectra in the Display menu to hide the selected spectra from view. A hidden spectrum cannot be seen in the spectral window; only its title appears in the title box list. The title is displayed using the font specified for the titles of hidden spectra in the Display options (available through Options in the Edit menu). The default font for displaying the titles of hidden spectra is italic. The order of titles is not affected when you hide a spectrum.

To make a hidden spectrum visible again, click its title in the title box list.

When you hide a selected spectrum, it is no longer selected. If any spectra remain in the window after you hide the selected spectra, one of the remaining spectra will be selected automatically.

1. Select the spectra.
2. Select Hide Spectra from the Display menu.

4.4.3 Full Scale

Select Full Scale from the Display menu.

The spectra are displayed at full scale as defined in the display range.

4.4.4 Display Range

You can set the X and Y axis display limits for newly created spectral windows by setting options in the Window options.

The spectra are then displayed using the limits you specified.

4.4.5 Automatic Full Scale

Automatic Full Scale in the Display menu automatically displays the spectra in the active spectral window full scale.

This is useful when you always want to view your spectra full scale.

Automatic Full Scale brings the highest data point of each spectrum (or the highest point of its annotations) to the top of its pane and the lowest data point of each spectrum (or the lowest point of its annotations) to the X- axis.

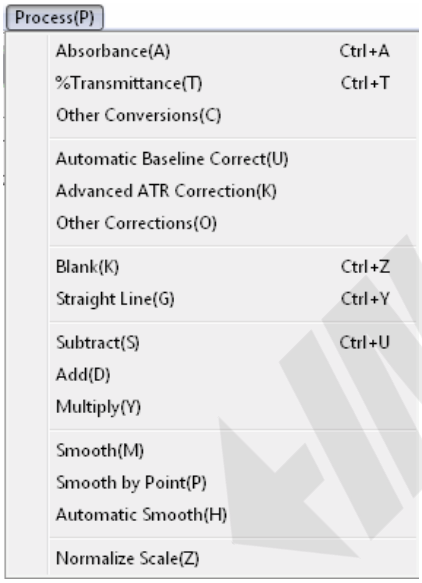
Display spectra full scale automatically

Select Automatic Full Scale from the Display menu.

To turn the command off, choose Automatic Full Scale from the Display menu when the check mark is present. The check mark will be removed.

4.5 Process

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



To do this...	**Use this command**...
Convert a spectrum to absorbance.	Absorbance
Convert a spectrum to % transmittance.	% Transmittance
Convert a spectrum to % reflectance	Other Convertions
Improve a baseline automatically.	Automatic Baseline Correction
Erase a spectral region.	Blank
Replace a spectral region with a straight line.	Straight Line
Subtract one spectrum from another.	Subtract
Add two spectra together.	Add
Multiply a spectrum by a number.	Multiply
Smooth sharp peaks in a spectrum.	Smooth
Smooth sharp peaks in a spectrum automatically	Automatic Smooth
Normalize the Y-axis scale of a spectrum.	Normalize Scale

4.5.1 Absorbance

Use Absorbance in the Process menu to convert spectra to absorbance units. Absorbance units show the amount of infrared energy absorbed by the sample.

The absorbance scale is useful in many areas of spectral analysis. You should normally convert spectra to absorbance before performing these tasks.

4.5.2 % Transmittance

Use % Transmittance in the Process menu to convert spectra to % transmittance units. These units show the relative amount of infrared energy transmitted through the sample.

Published infrared reference spectra are generally presented in % transmittance. It is easier to compare spectra when they are presented using the same Y-axis format. The % transmittance format is generally not as good as absorbance for manipulating data and performing quantitative analysis.

Percent transmittance at a frequency is defined by the equation

$$\%T = (S/B)*100$$

where S is the intensity of infrared energy through the sample and B is the intensity of infrared energy without a sample in place. B is called the background.

Convert spectra to % transmittance

1. Select the spectra.
2. Select % Transmittance from the Process menu

4.5.3 Other Conversions

Use Other Conversions in the Process menu to convert spectra to the following units.

Y-axis units:	**X-axis units:**
% Reflectance units	wavenumbers
Log (1/R)	wavenumbers
Kubelka-Munk	wavenumbers

4.5.3.1 % Reflectance

Select % Reflectance to convert spectra collected using a reflection technique to % reflectance units (see the following example. These units show the amount of infrared energy reflected from the sample. Some common reflection techniques include diffuse reflection (DR) and specular reflection (SR). Percent reflectance at a frequency is defined by the equation

$$\%R = (I_S/I_B) \times 100$$

Where I_S is the intensity of infrared energy reflected from the sample and I_B is the intensity of infrared energy passing through the reflection accessory with a reference sample, usually a mirror for SR, powdered potassium bromide (KBr) or chloride (KCl) for DR, or simply the open crystal for ATR. I_B is called the background.

4.5.3.2 Log (1/R)

Select Log (1/R) to convert reflection spectra to log (1/R) units. These units show the amount of infrared energy absorbed by the sample in a reflection experiment. You can convert spectra collected using the specular reflection (SR) and diffuse reflection (DR) techniques. Displaying these spectra in log (1/R) units is useful for identifying the technique used to obtain the data. The log (1/R) value at a frequency is defined by the equation

Log (1/R) = log (100/%R)

where %R is the % reflectance value of infrared energy at the same frequency. Displaying a reflectance spectrum in log (1/R) units is useful because there is often a linear relationship between the concentration of a component in a sample and the measured log (1/R) value.

Log (1/R) for reflection measurements is equivalent to absorbance in transmission measurements.

4.5.3.3 Kubelka-Munk

Select Kubelka-Munk to convert % reflectance spectra collected using the diffuse reflection (DR) technique to Kubelka-Munk units. Since these units are similar to absorbance units, the Kubelka-Munk format is useful for searching diffuse reflectance spectra against absorbance spectra in commercially available libraries. (Kubelka- Munk spectra are actually searched in absorbance.)
Due to pathlength variation, in many cases the concentration of samples run using the diffuse reflection technique do not vary linearly with log (1/R) (which is the equivalent of absorbance for reflection measurements). The Kubelka-Munk scale was developed to provide a more linear relationship with respect to concentration.

When you develop methods for determining component concentrations in sample mixtures, you can use spectra in log (1/R) or Kubelka-Munk units. Kubelka-Munk units are normally preferred because they eliminate any wavelength-dependent specular reflection effects, which reduce the accuracy of the analysis.
However, the Kubelka-Munk model is accurate only if these criteria are met:

- You are using high quality DR spectra.
- The sample is diluted with a non-absorbing matrix material

such as KBr.

- The sample concentration is low (about 1% sample to 99% matrix by weight).
- The sample and matrix material are finely ground (a particle size of 2 to 5 micrometers is recommended).
- The mixture is uniform in particle size and composition.
- The sample thickness must be at least 3 mm.

If these criteria are not met, use log (1/R) units instead of Kubelka-Munk, or see which scale gives a more linear response.

The Kubelka-Munk value at a frequency is defined by the equation KM = $\frac{(1-R)^2}{2R}$, where R is the reflectance intensity of the sample divided by the reflectance intensity of the standard.

4.5.4 Automatic Baseline Correction

Automatic Baseline Correction in the Process menu lets you automatically correct the tilted baseline of the selected spectra, with the baseline points selected by the software.

If a baseline is not just tilted but also has other undesirable characteristics, correct it using Baseline Correct.

Correct baselines automatically

1. Select the spectra whose baselines you want to correct.
2. Select (with the region tool) or display (with the view finder) the spectral region in which you want the baselines corrected.
3. Choose Automatic Baseline Correct from the Process menu.

4.5.5 Advanced ATR Correction

Advanced ATR Correction in the Process menu allows you to process an ATR spectrum to be more representative of a transmission spectrum. As the sampling depth is relative to the wavelength of light, the longer wavelengths produce a higher absorbance compared to the shorter wavelengths and hence, need to be corrected.

Correct ATR Spectrum

1. Select the ATR Spectrum to be corrected.
2. Select Advanced ATR Correction from the Process menu.
3. Select the crystal used in the measurement and also input the angle of incidence, number of reflections and index of refraction of the sample.
4. Click OK, and the corrected spectrum will be displayed in the window and will be automatically selected.

4.5.6 Other Corrections

Other correction modes are available by selecting Other Corrections in the Process menu.

To correct a spectrum:

1. Select the spectrum to be corrected.
2. Select Other Corrections from the Process menu.
3. Select the way of correction i.e. ATR or Kramers-Kronig
4. Click OK, and the corrected spectrum will be displayed in the window and will be automatically selected.

4.5.7 Blank

Use Blank in the Process menu to delete the data points in the selected spectra in order to do some data processing. Once exit Blank mode, spectrum will be restored.

To blank a spectrum:

1. Select the spectrum.
Use the region tool to select the target spectral region.

2. Choose Blank from the Process menu.
The spectrum you selected is erased.

3. Restore
When exit Blank mode, the erased spectrum is displayed again.

4.5.8 Straight Line

Straight Line in the Process menu lets you replace the selected region of the selected spectra (or the displayed region if no region is selected) with data points that form a straight line. Use Straight Line to remove unwanted spectral features such as totally absorbing bands in order to improve the appearance of a spectrum.

Don't use Straight Line to replace spectral region that contain important spectral information.

To replace a spectral region with a straight line:

1. Select the spectrum that contains the target spectral region.
2. Use the region tool to select the target spectral region.

If you do not select a region, the entire displayed region will be replaced with a straight line.

3. Select Straight Line from the Process menu.
A straight line is drawn between the two data points at the limits of the selected spectral region.

4.5.9 Subtract

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

When you use Subtract to subtract one spectrum from another, the software calculates data point by data point the difference between the two.

The Beer-Lambert law tells us the spectrum of a sample that is a mixture of two materials (say part 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 sample spectrum, the result spectrum is of the other pure component (A). This is expressed by the equation:

(A + B) - B = A.

In most cases components do not have the same concentration and so their intensities do not match so spectra are not subtracted data point by data point. For example, a mixture may be made up with 20% component A and 80% component B. Only after scaling a reference spectrum of part B so that its intensities match those in the sample spectrum, then a clean subtraction can be made leaving only peaks due to component A.

The subtraction looks like the following equation:

Sample - Reference * Factor = Result

You determine the subtraction factor interactively by watching the changes in the common peaks as you change the factor. The ideal factor is one which produces zero 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.

Subtract a spectrum from another spectrum:

1. **Select the two spectra on which you want to perform the subtraction**

First select the spectrum from which you want to subtract spectral features; this is the sample spectrum. Then select the spectrum with the features you want to subtract from the sample spectrum; we will call this the reference spectrum.

Select the spectra from the drop down list above the spectra. Either drag the mouse or hold down the Control key when selecting the second spectrum.

Important: The spectra must be converted from %Transmission to Absorbance mode.

2. Choose Subtract from the Process menu

The Subtract window appears with the sample spectrum displayed in the top pane and the reference spectrum below it.

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

If the spectra do not have the same resolution, the spectrum with the higher resolution will be temporarily reduced to match the resolution of the other spectrum. The subtraction operation will take longer in this case.

The spectral region displayed in the Subtract window is the same region that was displayed when you chose Subtract. To display a different region of all the spectra, use Display Range. The difference spectrum is displayed full scale in the bottom pane. This spectrum is the result of subtracting the reference spectrum from the sample spectrum using the subtraction factor shown to the left of the result.

To expand or contract the Y-axis of the difference spectrum, click the buttons to the right of the bottom pane. Expanding the spectrum helps you see small features.

Each time you click the Expand button, the scale of the Y-axis doubles.

Each time you click the Contract button, the scale of the Y-axis is reduced by one-half.

If you want to reverse the order of subtraction, click the double-arrow to the right of the spectra. The order of the spectra is reversed and the new difference spectrum is displayed in the bottom pane.

3. If you are not satisfied with the result, try changing the subtraction factor.

The current factor was calculated using the spectral data displayed when you selected Subtract. If you change the factor, the new spectrum will be automatically displayed in the bottom pane. There are two ways to change the factor: by using the scroll bar or by typing a new value.

To change the factor using the scroll bar, drag the scroll box or click the scroll to a position. The current upper and lower limits of the scroll bar range appear near at the top and bottom respectively.

The factor is displayed between the limits. To increase or decrease the range of the scroll bar, choose Crude regulation or Fine regulation. When Crude is selected, the range is approximately doubled. When Fine is selected, the range is approximately halved. Choosing Crude or Fine does not

change the current value of the subtraction factor displayed next to the scroll bar; only the number of decimal places in the factor setting may be affected.

The scroll bar by default uses Crude regulation.

To change the factor by typing a new value, click Coefficient.
In the dialog box that appears type a new coefficient in the text box and then select OK, or choose Cancel if you don't want to change the factor.

4. When satisfied with the resultant spectrum, place in a workspace.

To do this, select the desired option from the window selection drop down box near the top of the Subtract window and then choose Add or Replace. The title of the spectrum will be "Subtraction Result."

4.5.10 Add

Use Add in the Process menu to add together two spectra that have the same Y-axis unit. When spectra are added, each data point of one spectrum is added to the corresponding data point of the other spectrum.

Add a spectrum to another:

1. Select the two spectra you want to add together.

(Hold down the Control key when you select the second spectrum.) The spectra must be in the same spectral window. If they are not, first copy and paste one of the spectra into the window that contains the other.

2. Choose Add from the Process menu.

The spectra are displayed the same window as the subtract function. For a detailed description please refer to 4.5.9 Subtract. Once the spectra are added together and the result is displayed in the bottom of the window and then place in the same window or export to a new window.

4.5.11 Multiply

Use Multiply in the Process menu to multiply each data point in a spectrum by a number of your choice.

Multiply a spectrum by a number:

1. Select the spectrum that you want to multiply.

2. Select Multiply from the Process menu.

The Multiply dialog box requests the number to be used.

3. Type a number in the text box.

4. Select OK.

The spectrum is multiplied by the number you entered and displayed as a new spectrum in the same spectral window.

4.5.12 Smooth

Use Smooth in the Process menu to improve the appearance of the selected spectra by smoothing the high-frequency components of the spectral data. Smoothing is useful for improving the appearance of peaks obscured by noise.

If you want to smooth spectra manually, specify the degree of smoothing (setting the number of points), use Smooth. An automatic smooth option often gives a satisfactory result and is faster than a manual smooth.

The degree to which a spectrum is smoothed depends on the number of points used in the smoothing process. If you smooth more than one spectrum at the same time, all the spectra must have the same data point spacing.

Smooth a spectrum:

1. Select the spectra.

2. Select Smooth from the Process menu.

The Smooth dialog box appears.

3. Select the desired number of smooth points from the drop-down list box.

The options are: five points' cubic smooth, seven points quintic smooth and Savitzky-Golay.

4. Select OK.

4.5.13 Automatic Smooth

Use Automatic Smooth in the Process menu to improve the appearance of the selected spectra by automatically smoothing the high-frequency component of the sample data. Smoothing is useful for improving the appearance of peaks obscured by noise.

To automatic smooth:

1. Select the spectra.

2. Choose Automatic Smooth from the Process menu.

4.5.14 Normalize Scale

Use Normalize Scale in the Process menu to change the Y- axis scale of the selected spectra to a "normal" scale in which the Y values of the data points range from 0 absorbance units

for the lowest point to 1 absorbance unit for the highest peak (for an absorbance or absorbance-like spectrum) or from 10% to 100% transmittance (for a transmission or transmission-like spectrum).

In a transmission experiment, a thick sample of a material absorbs more infrared energy than a thin sample, resulting in greater peak heights. Normalizing the spectra compensates for this path length effect and lets you compare their peak heights.

In the case of an absorbance spectrum, Normalization first shifts the spectrum vertically to bring the lowest Y value to 0 absorbance, regardless of whether the lowest value is currently above or below. The software then multiplies the spectrum by a scaling factor to make the highest value 1 absorbance unit.

In the case of a transmission spectrum, the command first shifts the spectrum vertically to bring the highest Y value to 100 %T, regardless of whether the highest value is currently below or above 100%. The software then multiplies the spectrum by a scaling factor to make the lowest value (largest spectral feature) 10 %T.

Normalize a spectrum:

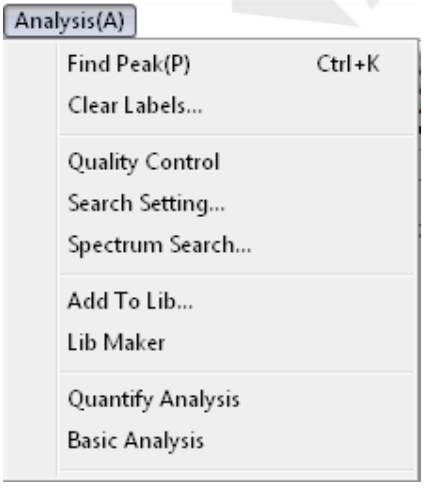
1. Select the spectra.

2. Choose Normalize Scale from the Process menu.

The normalized spectrum will be displayed in the current spectral window.

4.6 Analysis

Use the commands in the Analyze menu to obtain information from collected spectra.



The primary use of the commands is summarized in the following table:

To do this...	**Use this command**...
Identify peak locations in a spectrum.	Peaks
Remove peak locations in the specified area of a spectrum	Clear Labels
Compare samples against standards	Quality Control
Specify how to perform a spectral search	Search Setting...
Identify an unknown material by searching spectral libraries.	Spectrum Search...
Add current spectrum into the library	Add To Lib...
Open library maker	Lib Maker
Measure unknown sample concentration with known standard samples	Quantity Analysis
List functional group and chemical bond	Basic Analysis

4.6.1 Find Peak

Use Find Peak in the Analysis menu to identify a peak location in the spectrum.

The command searches for peaks whose Y values exceed a specified threshold value and then labels them with their X values.

By adjusting the sensitivity of the peak searching operation, you can find the spectral features you are interested in without labeling noise and other unimportant features.

Click the Print button to print the spectrum and a table of the labeled peaks below it. The peaks are listed in the table in order of wavenumber position or Y value (intensity), depending on the order specified in the Process options (available through Options in the Edit menu).

4.6.2 Clear Labels

Using the Clear Labels in the Analysis menu lets you remove all the peak locations in the specified area of a spectrum. If the peak locations in more than one area need to be removed, repeat this function in each area. Only the interested peak locations info is left in the spectrum.

4.6.3 Quality Control (QC Compare)

Using the Quality Control feature in the Analysis menu allows you to compare the current spectrum against the library.

QC compare

1. Select the spectra.

2. Select Quality Control from the Analysis menu.

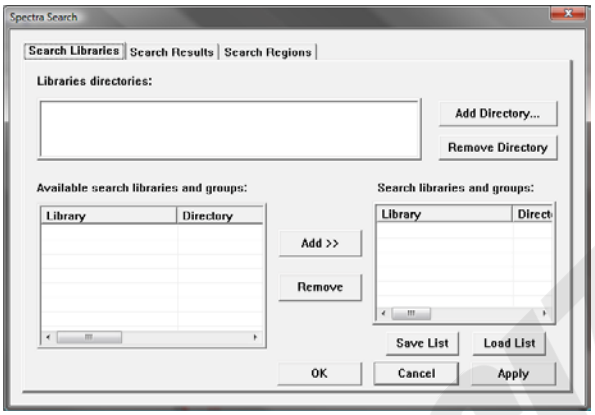
3. If the threshold value is changed, click Refresh button.

4.6.4 Search Setting

Using the Search Setting in the Analysis menu lets you define the settings for spectral searching. Once results are obtained and any required manipulation (e.g. subtraction) is completed, before conducting a search, check the search settings to optimize the searching performance.

4.6.4.1 Search Libraries

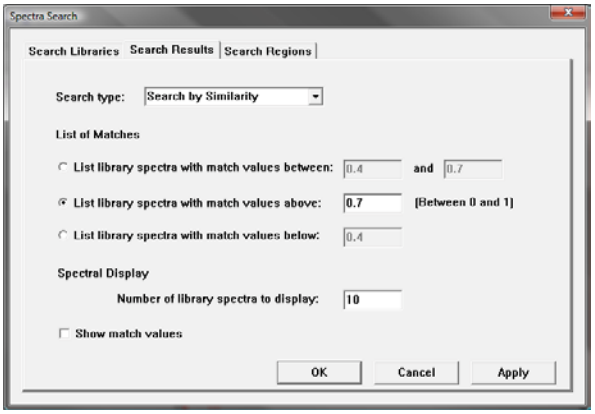
The Search Libraries tab contains the directories for which you can specify to search. You can also add or remove directories.



To specify or do this…	**Use this feature**…
Add a new library directory.	Add Directory
Remove a library directory.	Remove Directory
Add a new directory for searching directory.	Add
Remove a directory from the search list.	Remove
Save a specific list of directories for searching	Save List
Load a previously saved list of directories.	Load List

4.6.4.2 Search Results

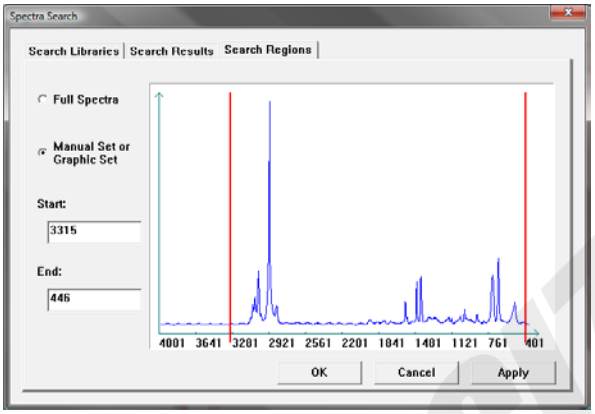
The Search Results tab provides options used to define the search parameters.



To specify or do this…	Use this feature…
Search by number of similar, similarity and variance.	Search type
Specify a search threshold.	List of Matches
Define the number library spectra to display.	Spectral Display
Display the matching values.	Show match values

4.6.4.3 Search Regions

The Search Regions tab lets you select either the full spectra for searching or a defined region for searching. Defining a region for searching can be done by either using the mouse to drag the region limits or input the region limits.



To specify or do this…	Use this feature…
Search using the full spectrum.	Full Spectra
Search a user defined region.	Manual Set or Graphic Set

4.6.5 Spectrum Search

Using the Spectrum Search feature in the Analysis menu allows you to identify an unknown spectrum. This function searches the libraries define in the Search Settings.

4.6.6 Add To Lib

Using the Add To Lib feature in the Analysis menu allows you to add the current spectrum into the library.
Smooth a spectrum:

Add a spectrum into library

1. Select the spectra.

2. Select Add To Lib from the Analysis menu.

3. Select library, input chemical name and click OK.

4.6.7 Lib Maker

Using the Lib Maker feature in the Analysis menu allows you to open a program for creating a spectrum library.

4.6.8 Quantity Analysis

Using the Quantity Analysis in the Analysis menu allows you to analyze the unknown sample concentration with known samples.

Quantity Analysis process

1. **Collect Standard Sample:** background will be collected first, then, you are reminded to put into standard sample. Once you get the standard spectrum, select the desired peak using a green cursor line. Then, enter the sample concentration and unit. Click **Calculate Curve Point.** Repeat above procedures to get required points, normally 5 to 6 points.

2. Select fitting equation: **Simple equation, Quadratic equation and Cubic equation** in **Construct Curve** area**.**

3. Click **Construct Curve** and a fitted curve is displayed on the left frame. The default coordinate mode: X-ABS and Y-Conc and this can be changed via coordinate mode option.

4. Click **Collect Pending Sample** to measure unknown sample spectrum. The desired peak can be same as standard sample automatically or fine adjusted manually.

5. Click **Calculate.** Alternatively, you can click **Calculate…** directly and input the known absorbance of sample.

6. The constructed curve can be saved by clicking **Save** button.

7. The saved constructed curve can be used by clicking **Open** button.

4.6.9 Basic Analysis

Using the Basic Analysis feature in the Analysis menu allows you to analyze the peak in a current spectrum.
There are two sensitivity adjustments: analysis sensitivity and peaking sensitivity. The lower the value, the higher the sensitivity. Click Refresh button to adopt the changed value. You can choose to print the selected analysis result or print all the results.

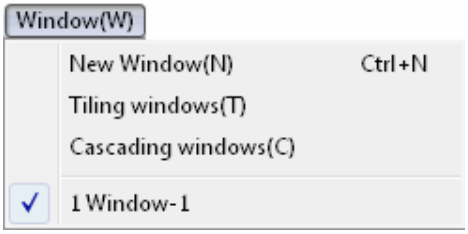
1. Select the spectra.

2. Select Basic Analysis from the Analysis menu.

3. If the sensitivity value is changed, click Refresh button.

4.7 Window

The Window menu includes commands for working with spectral windows on the screen. The primary use of each command is summarized in the following table:



To do this...	**Use this command**...
Create a new spectral window.	New Window
Display spectral windows in a tiled arrangement.	Tiling windows
Display spectral windows in a layered arrangement.	Cascading windows

4.7.1 New Window

Use New Window in the Window menu to create a new spectral window. The window becomes the selected window.

Create a new spectral window:

1. Choose New Window from the Window menu.

If Prompt for New Window Title is turned on in the Window options (available through Options in the Edit menu), a dialog box asks for a title for the new spectral window.

A new spectral window appears on the screen. Its appearance depends on the settings of the Window options (available through Options in the Edit menu).

4.7.2 Tiling windows

Use Tiling windows in the Window menu to resize and rearrange all of FTIR-650's spectral windows so that they fill the FTIR window without overlapping, like floor tiles. The windows are automatically resized and reshaped as needed to make them fit. Rearranging the windows in this way lets you see all of the spectral windows at the same time and lets you easily move between windows when there are many on the screen.

The title of every window is listed at the bottom of the Window menu. You can select any of these windows by selecting its title from the Window menu.

Tile spectral windows:
1. Select Tiling windows from the Window menu.

4.7.3 Cascading windows

Use Cascading windows in the Window menu to resize and layer all of FTIR-650's displayed windows and arrange them within the FTIR window so that their title bars are visible.

Cascade spectral windows:
1. Select Cascading windows from the Window menu.

4.8 Help

4.8.1 About FTIR

Select to display the version information about the software.

4.9 Toolbar

A toolbar is provided for quick accessing of functions for determining properties of spectra. These tools determine what function the mouse will take when analyzing a spectrum. To undo any functions just right click the mouse (except for peak search). Pictured below is the toolbar.

4.9.1 Selection

Selection is the default setting and it is used to select an area of interest of the spectrum (it will automatically zoom in on that area) and for selecting spectra for manipulation (e.g. subtraction).

4.9.2 Cursor

Cursor function places crosshairs on the spectrum at the point at which is selected by clicking the mouse. This function displays the X and Y coordinates of the selected point in a display bar below the spectrum. Once a point has been selected, use the left and right arrow keys to move along the spectrum to determine a feature coordinate (e.g. a peak).

4.9.3 Region

The Region function is used to determine a width of any spectral feature(s). It is best used when the feature has been isolated by using the selection tool. By clicking at one point then moving the mouse to obtain a second limit, the X coordinates and the width are displayed in the display bar below the spectrum.

4.9.4 Peaks

Please see 4.6.1 Find Peak

4.9.5 Height

Measure the height of a peak, corrected or uncorrected

4.9.6 Area

Measure the area under a peak, corrected or uncorrected

4.9.7 Annotation

Annotation tool is used for labeling features on a spectrum. Again it is best used after isolating the feature using the selection tool. Click on the point of interest and the X coordinate will be displayed in an input box. Type in the label for that point or if the X coordinate is desired just leave the input box. Right click to view the label; if you left click it will place another label. To undo the previous label, right click again.

4.9.8 Normalize Scale

Normalize the current spectrum

4.9.9 Search Setting

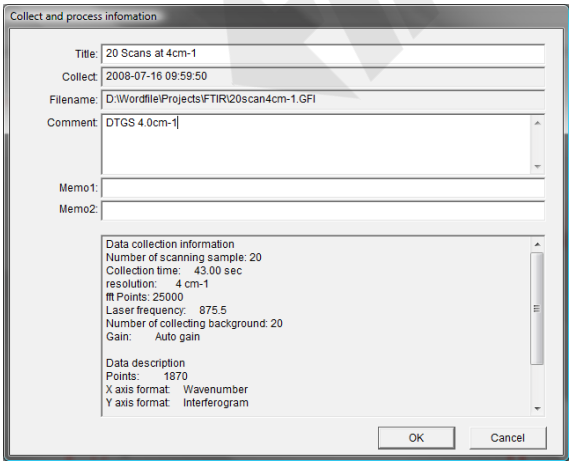
Shortcut to Search Setting

4.910 Spectrum Search

Shortcut to Spectrum Search…

4.9.11 Spectrum Information

Located next to the spectrum name in the drop down list, selecting Spectrum Information allows information about the spectrum to be input and saved with the spectrum for future reference. Data collection information is also provided for monitoring data collection performance.



4.9.12 Drop-down List

Clicking on the drop down list shows the list of current spectra in the current spectral window. This can be used to select hidden spectra, multiple spectra for manipulation (e.g.