Spectrum RX I
Routine Operations

Release History

Part Number	Release	Publication Date
0993 4217	A	December 1997
	B	March 2000

User Assistance
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Beaconsfield
Buckinghamshire
HP9 1QA

Printed in the United Kingdom.

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Warnings and Safety Information

Summary

The Spectrum RXI has been designed to comply with a wide variety of international standards governing the safety of laboratory equipment. In routine use, the Spectrum RXI poses virtually no risk to you. If you take some simple, common-sense precautions, you can make sure that you maintain the continued safe operation of the instrument:

DO make sure that the Spectrum RXI is properly connected to the electrical supply; in particular make sure that the ground (earth) is securely connected.

DO disconnect the electrical power cable before opening the main cover of the Spectrum RXI.

DO keep the Spectrum RXI dry. Avoid spilling liquid into the instrument, especially into the top of the display-screen housing, which contains a high-voltage supply. Clean all external spills immediately. If anything that is spilled enters the main body of the Spectrum RXI, switch off the power and call a Perkin-Elmer Service Engineer.

DO NOT stare into the laser beam. The Spectrum RXI contains a low power, visible (red) laser; momentary exposure to the beam is not dangerous, but deliberate, direct viewing of the beam along its axis could damage your eye.

DO NOT use a flammable gas to purge the Spectrum RXI. The Spectrum RXI contains a hot source, and a fire or explosion will result. Only use clean, dry, oil-free nitrogen or air to purge the instrument.

DO take care if you need to open the main cover of the instrument. The screen is a separate unit and must be removed before opening the cover.

DO read the more detailed information on safety in *Getting Started*.

Preface

This manual contains an overview of the Spectrum RXI and describes the features that you will require most frequently – such as collecting spectra, and viewing and processing them.

Using this Manual

This manual has seven chapters:

- **An Overview of the Spectrum RXI**: a description of the hardware, the screen, and memory locations, and some information about entering commands.
- **Collecting Spectra**: how to collect spectra and monitor, and how to set up the Scan options.
- **Viewing and Processing**: how to use all the viewing and processing features.
- **Printing and Plotting**: a description of the print and plot options, and how to print and plot.
- **Copying and Storing Data**: how to work with directories and files.
- **Methods**: how to use methods, and a description of those that are provided.
- **Index**

Conventions Used

All the documentation supplied with your Spectrum RXI use the following conventions to indicate various methods of entering commands:

- Keypad keys are referred to as *hard keys* and are represented by gray boxes. For example, scan.
- The top row of the keypad keys are called the soft keys. The function of the soft keys changes as you access different commands. Instead of permanent labels, soft keys have labels that appear on the screen. Soft keys are represented by white boxes: setup.
- Soft keys that execute their command immediately, without the entry having to be confirmed, are called *action keys*. Action keys are represented by black boxes: EXECUTE.
- Text that you type, or that appears on the screen is printed in **this type**: The cursor moves to the **from** field. Type **1020**.
- Typed commands for use in method/Obey files are printed in **this type**: **noise Y 4000 3750**

  In a representation of the format for such a command, only the key word is **bold**:

  noise x w1 w2

An Overview of the Spectrum RXI 1

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A Guided Tour of the Spectrum RXI FT-IR

The Perkin-Elmer Spectrum RXI FT-IR spectrometer (Figure 1-1) is a bench-top instrument that provides all of the following:

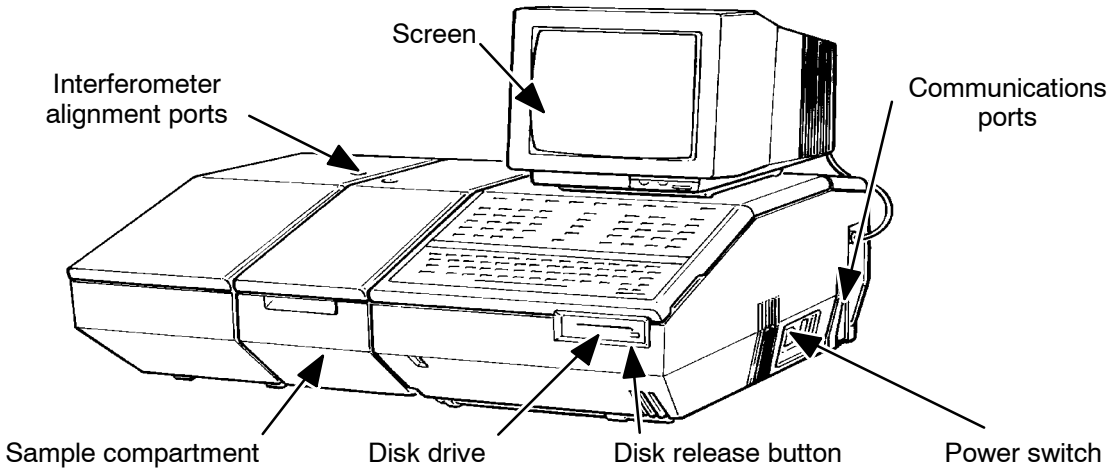


Figure 1-1 The Spectrum RXI

- A dedicated keypad for controlling the instrument and interacting with the software.
- A single-beam, purgeable, sample compartment. The Spectrum RXI can operate in ratio, single-beam, or interferogram mode.
- An optical system that gives you data collection over a total range of 7800 to 370 cm^{-1}, with maximum OPD resolution of 1 cm^{-1}.
- An LITA (lithium tantalate) mid-infrared detector as standard, and the option of using a PAS (photoacoustic detector).
- An electronics system based on the Motorola 68340 Integrated Processor. The Spectrum RXI has 32 KB of battery-backed memory, so that your customized methods and parameter settings are retained when the Spectrum RXI is switched off.
- Compatibility with output devices such as plotters and printers, including laserjets.

Sample Compartment

The sample compartment is located at the front of the Spectrum RXI, to the left of center. You open the sample compartment by lifting the cover using the recess at the front. Figure 1-2 shows the left- and right-hand sides of the interior of the sample compartment.

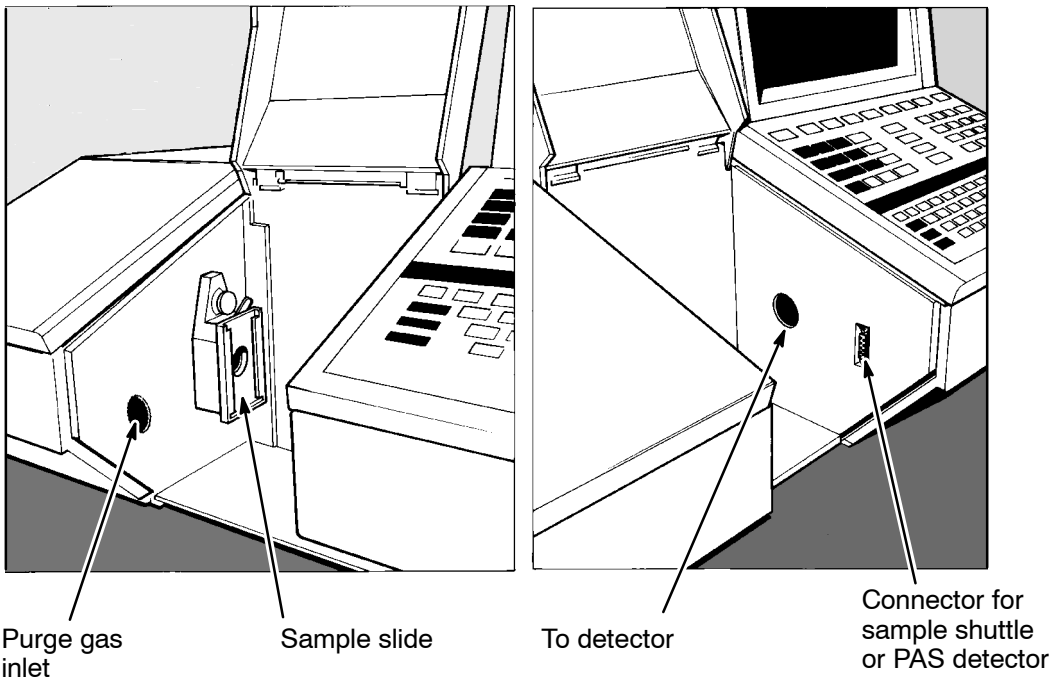


Figure 1-2 Interior of the Sample Compartment

- The infrared beam enters the sample compartment through an aperture on the left, behind the sample slide. After passing through the sample, it enters the detector area through an aperture in the right-hand side of the sample compartment.
- The inlet for purge gas is on the left-hand side of the sample compartment. It is connected to a tube that exits at the rear of the Spectrum RXI, on the left-hand side. (See *Purging the Spectrum RXI*, starting on page 2-41.)
- If you use an optional sample shuttle or photoacoustic detector, it plugs into the connector on the right-hand side of the sample compartment.

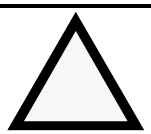
- The baseplate of the sample compartment is removeable, enabling you to use accessories that are mounted on a baseplate.
- The sample slide contains an alignment light that is used to align accessories; the lever on the sample slide enables you to switch the alignment light on and off. Make sure that you switch it off before scanning, otherwise it blocks the beam.
- You can use a wide range of sampling accessories in the Spectrum RXI, for example, diffuse reflectance, Horizontal Attenuated Total Reflectance (HATR), and specular reflectance.
- To achieve 1 and 2 cm^{-1} resolution, you need to use a J-stop (Jacquinot stop) when you collect spectra (this is discussed in the tutorials). A J-stop is an aperture in a metal plate that *slides* into the sample slide. The J-stops are supplied in the shipping kit. If you have worked through the *Tutorials*, you will already have used a J-stop; they are also described in this manual, starting on page 2-38.

WARNING

A portion of the laser radiation with a maximum power level of less than 0.4 mW may be accessed in the sample compartment. The laser is automatically switched off when the main cover of the Spectrum RXI is raised.

CAUTION

The sample compartment windows are composed of KBr, which, although coated, can be damaged by high levels of humidity. If you spill a liquid in the sample compartment, wipe it up quickly. When working with water-based samples open to the air, either purge the sample compartment or leave the cover open.



CAUTION

Relative humidity higher than 75% can damage the windows of the sample compartment. If you expect the humidity to exceed 75%, continually purge or desiccate the sample compartment.

Interferometer Alignment Ports

In the main cover, behind the sample compartment, are the Interferometer Alignment Ports (Figure 1-1 on page 1-1). By removing the two inserts, you access the screws that enable you to adjust the interferometer and maximize the energy throughput. The procedure for *Adjusting the Interferometer* is in *Getting Started.*

Screen

A high-resolution, 16-color, standard SVGA screen is supplied for displaying both results and information about the status of the instrument. (The sixteen colors can be selected from a palette of more than a quarter of a million colors.)

The screen of the Spectrum RXI is divided into three regions (which are described in the section that starts on page 1-13):

- *title bar* – the top line of the screen;
- *display area* – where information is displayed in one of three possible formats — graphics, text (the scroll buffer), or tables;
- *user interaction area* – which contains command lines and soft keys.

The screen includes controls for power, brightness and contrast.

Keypad

You use the Spectrum RXI keypad to enter commands, view and process displayed spectra, and perform calculations. The keypad includes both dedicated function keys and programmable soft keys. You usually control the Spectrum RXI from the keypad, although you can also control it from a PC or an external keyboard. (For more information about *Entering Commands*, see page 1-23.)

The keys are pressure-sensitive. When you press them, a beeper sounds; soft keys in Setup enable you to set the volume of this beeper. (See the *Beeper* option in *User Preferences* in *Advanced Operations.*)

The keypad has two main regions:

- the top is the spectroscopic keypad, which you use to control the Spectrum RXI;

- the bottom is similar to the keypad you find on most PCs.

The keypad is illustrated in Figure 1-3.

The keys in the spectroscopic keypad are in four groups:

- along the top are the soft keys, with the **setup** and **help** hard keys on either side. The soft keys have different functions as you access different commands. Instead of permanent labels, soft keys have programmed labels on the screen.
- at the right is the block of keys you use most frequently. These are the keys that enable you to collect, view, copy, print, and plot spectra.
- in the center are the data-processing keys. These keys enable you to improve the appearance of your spectra for presentation, or comparison with your standard spectra.
- at the left are the calculation keys. These enable you to apply mathematical functions to spectroscopic data. They are generally most useful to the advanced user.

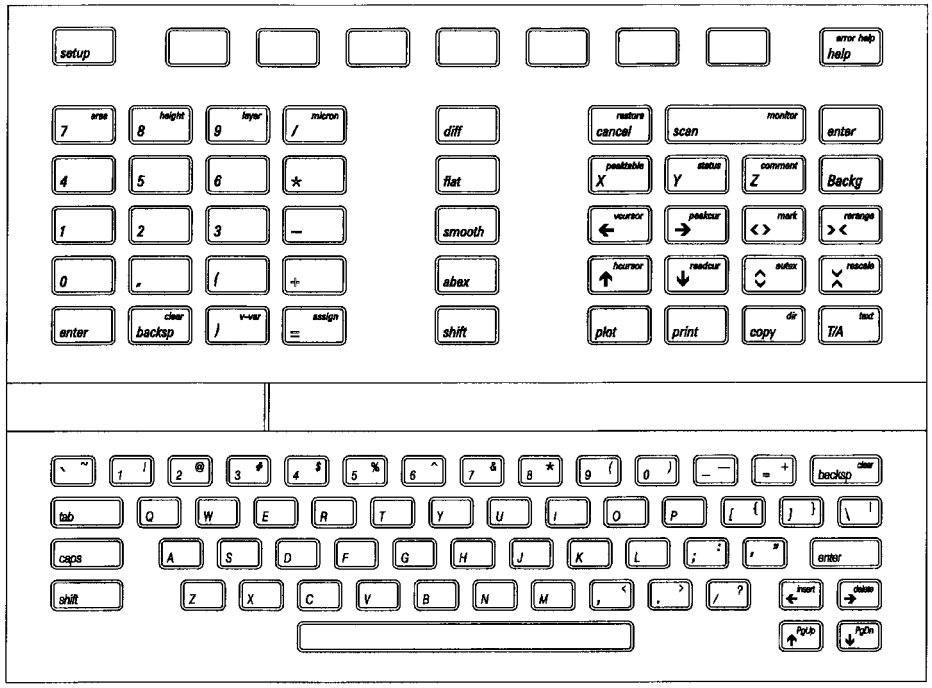


Figure 1-3 The Keypad of the Spectrum RXI

Disk Drives

A floppy disk drive is available for the Spectrum RXI, which can be used to store copies of spectra and methods for future use. You can also copy the spectra that you have on disk back into the data regions. This provides more flexibility in data handling and storage. (*Copying and Storing Data* are described later in this manual. In *Storing Spectra* in *Tutorials*, you learn to store a spectrum on a floppy disk, and retrieve the spectrum and copy it into a spectrum region.)

You can save instrument configuration files to disk. These files (see page 1-14 of *Advanced Operations*) enable you to save all of the settings of your Spectrum RXI, including the methods stored in the method regions, to a file.

Floppy drive

The floppy disk drive is located to the right-hand side of the Spectrum RXI, beneath the keypad; it takes 1.44 MB and 720 MB, 3.5 inch disks, and is IBM-compatible. The disk drive is horizontal. To insert a disk, hold it by the edge next to the label, and insert it in the drive with the label at the top.

Power Switch and Communications Ports

The power switch, AC power cable connector, and communications ports are on the right-hand side of the Spectrum RXI, as you look from the front (Figure 1-4). The power switch is marked I/O (on/off).

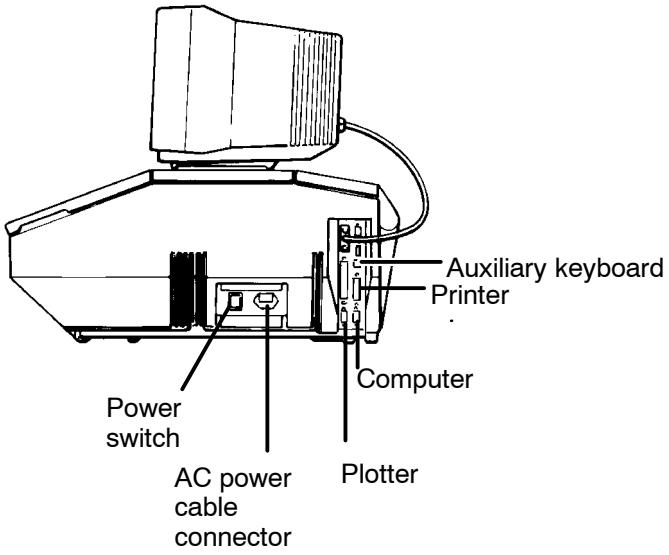


Figure 1-4 Connectors on the Side Panel

The communications ports enable you to connect external devices, for example printers, plotters and PCs, to the Spectrum RXI (Figure 1-5). To find out how to connect and configure external devices, see *Communicating with Other Devices* in *Advanced Operations*.

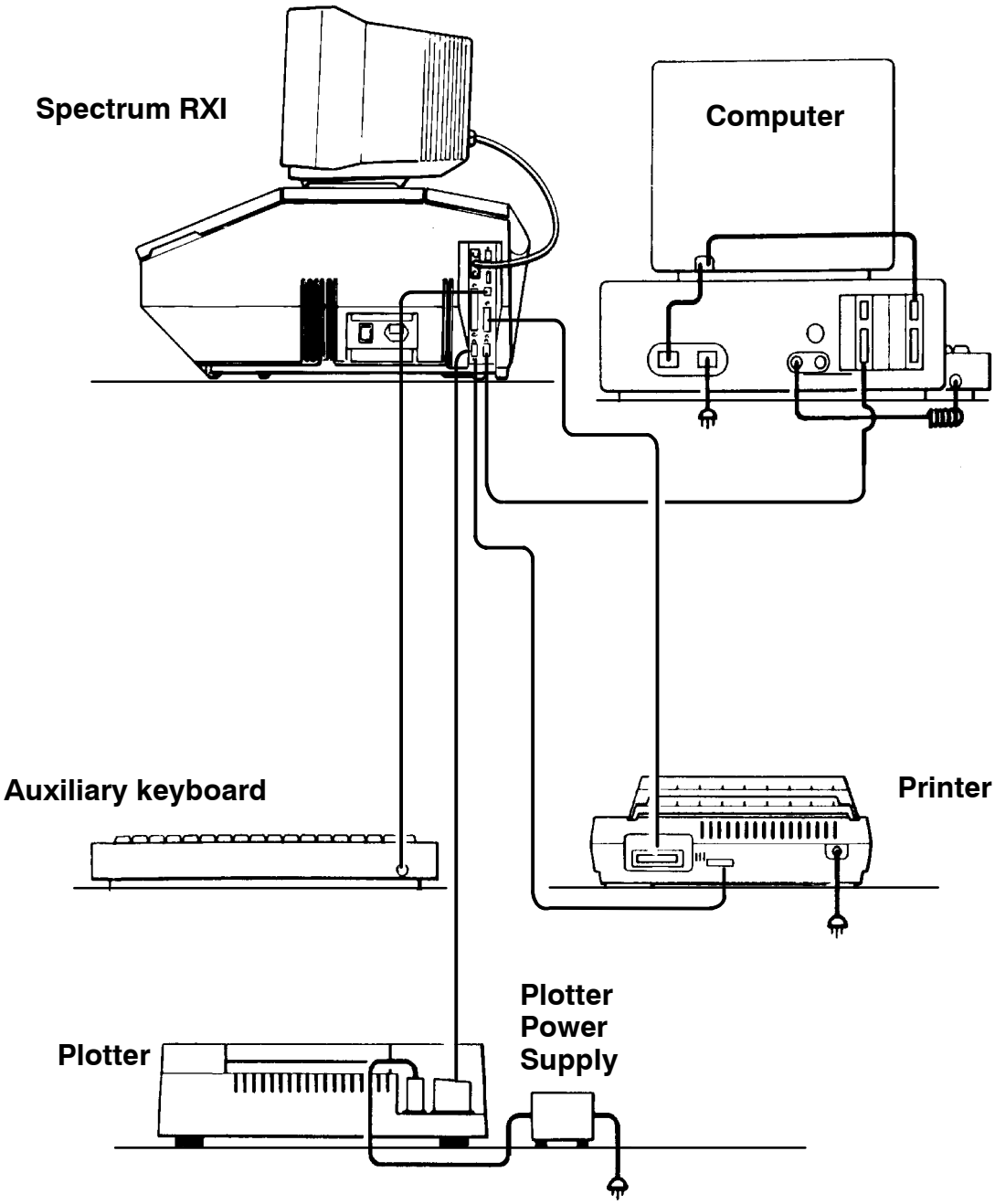


Figure 1-5 Connecting Peripheral Devices to the Spectrum RXI

Diagnostic Signal Lights

Next to the communications ports is a set of six lights (Figure 1-6). Five of these lights are lit when the Spectrum RXI is switched on. If any of the five marked lights are out, contact your local Perkin-Elmer Service department.

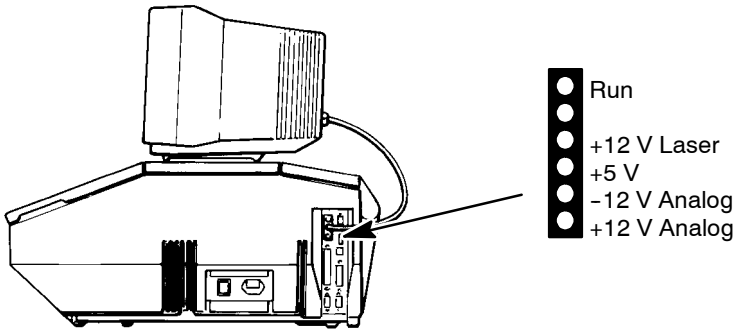


Figure 1-6 Diagnostic Signal Lights

Optical System

Usually the cover of the Spectrum RXI is closed, but to perform most maintenance tasks, you have to open the cover of the Spectrum RXI and prop it open (for instructions, see *Maintenance* in *Advanced Operations*). When you do this, a safety interlock automatically switches off the power. Under the cover is the optical system of the Spectrum RXI.

Consistent, reliable performance in single-beam, ratio, or interferogram mode is achieved by having few moving or adjustable parts, and by extensive insulation of the optical system from the effects of heat, humidity, and vibration.

Stability of the optical system components

The optical bench *floats* on vibration reducing mounting pads, which protect the optical system from bench shocks, enabling you to use the keypad while scanning.

The entire optical system is purged and sealed at the factory. A supply of desiccant placed within the system removes any water vapor and carbon dioxide that may enter.

Rigid insulating material encloses the infrared source (Figure 1-7), which is a heated wire. This insulation reduces vulnerability to shocks and also convection of heat.

The scan speed of the moving mirror in the interferometer defaults to the appropriate value for the detector. The swinging-arm interferometer has only one moving part; counterbalancing makes it almost immune to shocks. The design of the interferometer makes it immune to tilt and shear.

KBr windows separate the sample compartment from the purged optical system. You can purge the sample compartment with dry air or nitrogen. Either one removes water vapor; however, nitrogen is preferable because it also removes atmospheric carbon dioxide.

WARNING

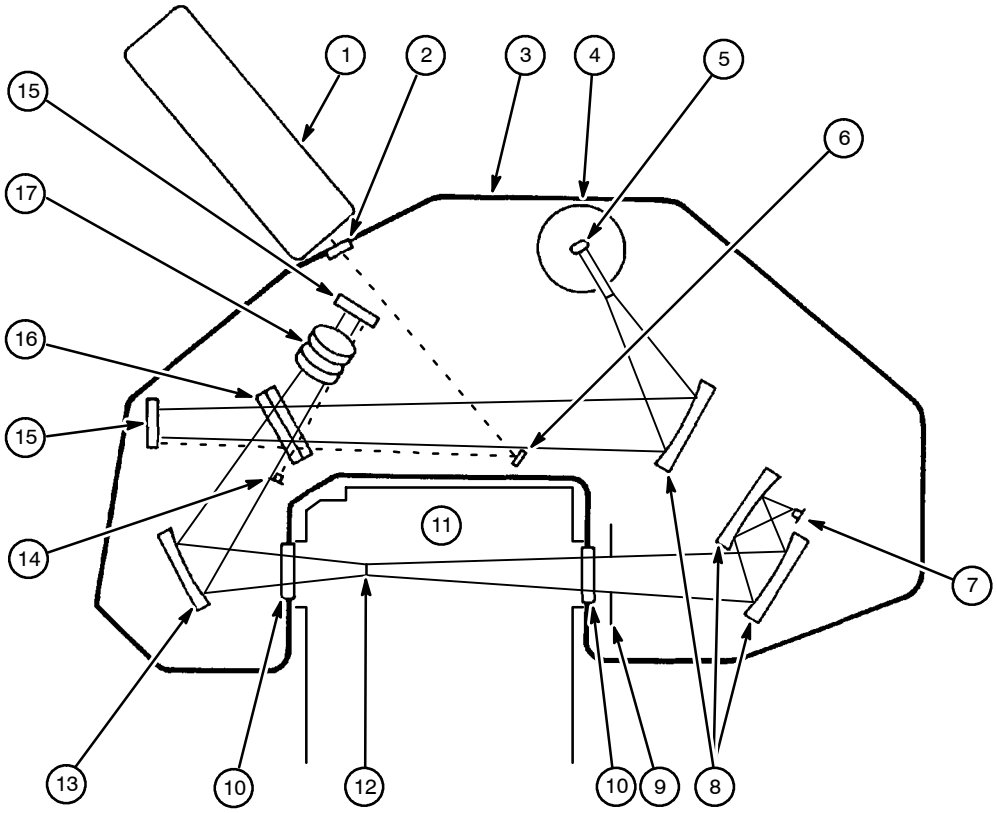
Do not use a flammable gas to purge the Spectrum RXI. The Spectrum RXI contains a hot source, and a fire or explosion will result. Only use clean, dry, oil-free nitrogen or air to purge the instrument.

Optical path

Figure 1-7 illustrates the optical path in the Spectrum RXI. The infrared beam begins at the source coil; a concave, off-axis mirror collimates the beam from the source and directs it to the interferometer.

The beam from a HeNe (helium neon) laser follows the infrared beam through the interferometer. (As shown in Figure 1-7, the laser itself is outside the purged area, to minimize buildup of heat.) The Spectrum RXI uses the laser beam to track the distance the moving mirror travels (the optical path difference) and to determine when to record a data point.

The concave mirror focuses the beam from the interferometer into the sample compartment. From the sample compartment, the beam travels through an optical stop to a pair of concave mirrors that focus the beam onto the detector.



1 HeNe laser
2 Glass window
3 Purge cover
4 Shield
5 Source coil
6 Adjustable laser mirror
7 IR detector
8 Fixed concave mirrors
9 Optical stop
10 KBr window
11 Sample compartment
12 IR beam focus
13 Adjustable concave mirror
14 Laser fringe detector
15 Interferometer flat mirror
16 Beamsplitter
17 Interferometer scan mirrors (2)
—— IR beam
- - - Laser beam

Figure 1-7 The Optical Path in the Spectrum RXI

Accessories and Other Devices

Although the Spectrum RXI is a complete, self-contained system for collecting, viewing and processing spectra, you can expand it to meet your needs by adding accessories or connecting other devices.

The Spectrum RXI has a Centronics interface and a serial port, to which you can attach a printer, a plotter, or both. You can also attach a computer to the Remote PC port of the Spectrum RXI; this enables you to use external data-processing software. Perkin-Elmer Spectrum for Windows software, which is available for your PC, can be used to control the Spectrum RXI.

To obtain a brochure that describes the accessories and other devices that are available for the Spectrum RXI, contact your local Perkin-Elmer sales office or agent.

Screen

The screen of the Spectrum RXI is divided into three regions (Figure 1-8), which are described on the following pages:

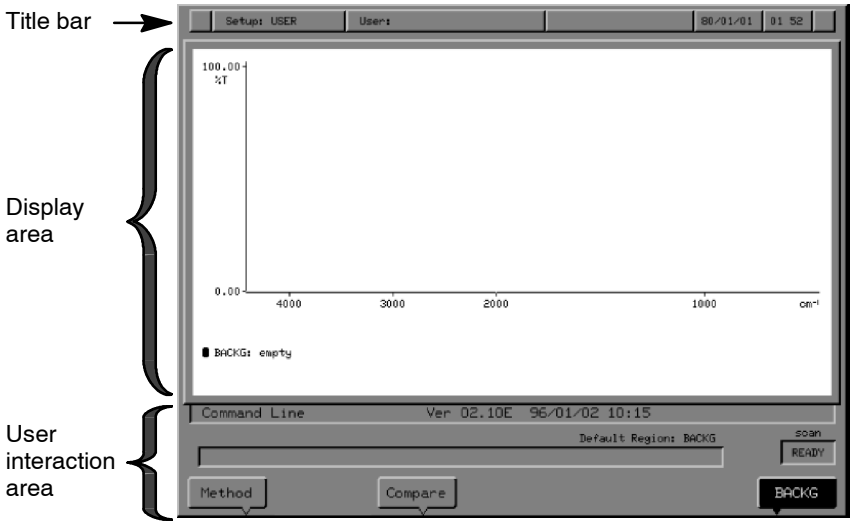


Figure 1-8 The Screen of the Spectrum RXI

Title Bar

This is the top line of the screen. In the title bar, the following information is displayed (Figure 1-9):

Figure 1-9 The Title Bar of the Spectrum RXI Screen

- **User** – the name of the user, which you enter yourself. The user-name is saved with each spectrum that is collected, and it appears in the Status information for the spectrum, and in the captions of plots. To change the name, follow the instructions on page 1–7 of *Advanced Operations.*
- **Setup** – there are three types of setup:
  - **User** – a setup that you define using the various setup options;
  - **Factory** – the default factory setup**;**
  - **Temporary** – the factory setup, but with changes that you have made.
- instrument identification – defaults to the message **Serial No: ######**, but may be customized to any 18-character message that you wish to use. To change the message, follow the instructions on page 1–8 of *Advanced Operations.*
- the date, in the format year/month/day, and time. To set the date or time, follow the instructions on page 1–2 of *Advanced Operations.*

Display Area

The display area of the Spectrum RXI screen is never empty; it always displays information, in one of three possible formats — graphics, text (the scroll buffer), or tables.

Graphics

Usually, the display area contains graphics, consisting of one or more spectra (or interferograms), as shown in Figure 1-10. Graphics are always displayed when the Spectrum RXI is first switched on.

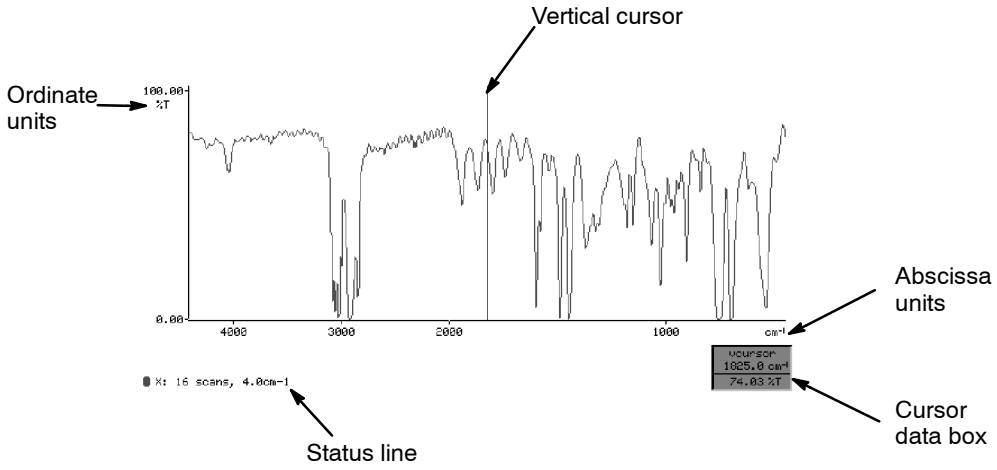


Figure 1-10 The Graphics Display

To return to graphics when a text screen is displayed:

- Press ***text***.

  or

- Press any View Key (see Chapter 3, *Viewing and Processing*).

  or

- Start a command that uses or collects spectral data (for example, Smooth or Scan).

Note the following features of the graphics display:

- *Abscissa and ordinate*: Every time the graphics display reappears, its ordinate scale (on the vertical axis, in units of %T or A) and abscissa range (on the horizontal axis, in units of cm^{-1} for spectra) are set just as they were when graphics were last displayed. For example, if you expand the spectrum in Figure 1-10 so that only the range from 3000 to 1000 cm^{-1} is on the screen, then switch the graphics off, the next time the graphics appear *for any reason*, the range is still 3000 to 1000 cm^{-1}.
- *Status line*: The spectra displayed on the graphics screen are stored in the Spectrum RXI in four memory locations, called *spectrum regions*. These spectrum regions are called X, Y, Z, and Backg. The status line in Figure 1-10 reports that the spectrum in region X is displayed, and gives the number of scans and the resolution at which the spectrum was collected. The colored mark to the left of the region name identifies the color of the related spectrum on the display; this is particularly important when you have more than one spectrum displayed.
- *Scale change*: Notice that the distance from 3000 to 2000 cm^{-1} in Figure 1-10 is half the distance from 2000 to 1000 cm^{-1}. This is because the optional 2:1 scale change at 2000 cm^{-1} is switched on. To switch the scale change on and off, see page 3-12.
- *Cursors*: The vertical and horizontal graphics cursors and their accompanying data box are switched on and off using ***vcursor***, ***peakcur***, and ***hcursor***.
- *Cursor data box:* This is at the bottom right of the screen. The abscissa position (wavenumber) of the cursor is reported under the label **vcursor**; the ordinate value (%T) at that position is reported in line with the spectrum status line. When more than one spectrum is displayed, the cursor data box extends and the additional ordinate values are also reported.

Scroll buffer

The scroll buffer is a region of memory used to store the previous 24 lines of input, for example scan, view, and plot commands, and the output of alphanumeric results (such as cursor values, status reports, and error or warning messages). An example of a scroll buffer – a text display – is shown in Figure 1-11. You may find it useful to refer to the scroll buffer for information about the sequence of events leading to a particular result. When you run a method, the scroll buffer displays instruction messages and results.

To view the scroll buffer, press **status** or **text**. Pressing **status** displays the scroll buffer, and each time that you press **status** , information about the data in the spectrum region or regions currently on the screen is added to the scroll buffer; pressing **text** toggles between the graphics display and the scroll buffer.

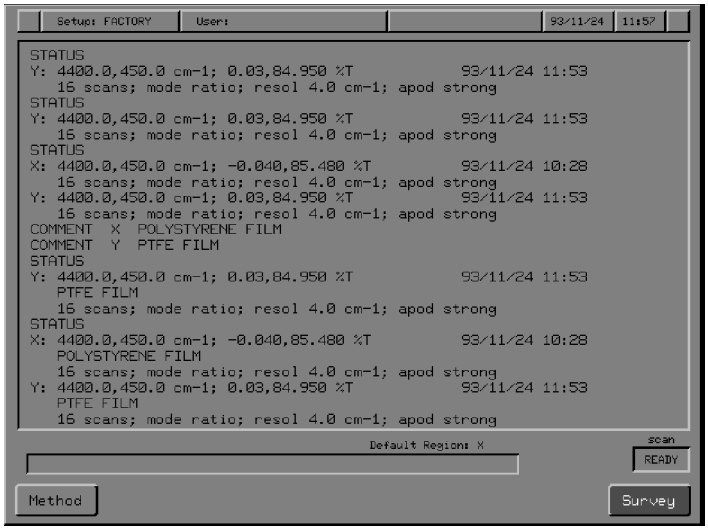


Figure 1-11 The Scroll Buffer

Tables

During some user interactions, the Spectrum RXI displays tables to provide you with information. Figure 1-12 is a table taken from the View options of Setup: it lists the current settings of the View options.

You cannot switch tables on or off, and you cannot switch on graphics or text while a table is displayed.

Figure 1-12 Table Display from the View Options of Setup

Sleep Mode

When the screen display does not change for a long time, it can leave a permanent trace on the screen. To prevent such damage, the screen of the Spectrum RXI goes into sleep mode when a key has not been pressed for 15 minutes. The screen is blank except for the message:

Press Enter to continue

or

Time to change desiccant: see MAINTENANCE chapter of manual
Press Enter to continue

When you are ready to resume working with the Spectrum RXI, press ***enter***. The previous display returns unchanged.

User Interaction Area

The appearance of the user interaction area depends on whether the Spectrum RXI is waiting for a command, or you are entering a command, or a command is being executed. This section tells you what to expect in each of these situations.

Ready For Next Command

Figure 1-13 shows the user interaction area as it appears when you first switch on the Spectrum RXI and when all options are at their factory-default settings. The Spectrum RXI is waiting for you to enter a command (for more information about entering a command, see page 1-23). This is called *Ready For Next Command*, and it is indicated by:

- the text cursor at the beginning of the command line;
- the box around the entire command line.

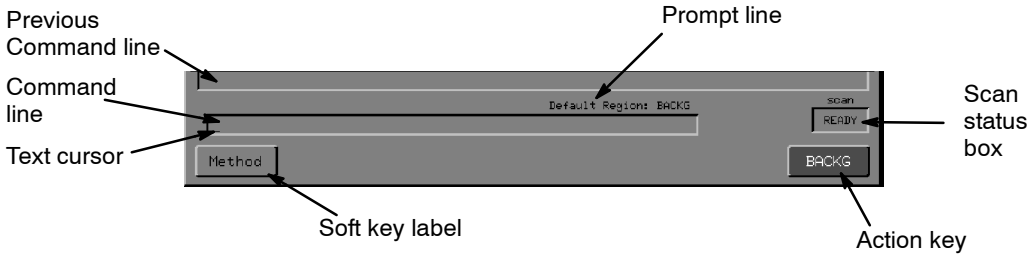


Figure 1-13 The User Interaction Area at Ready For Next Command

The features of the user interaction area at Ready For Next Command are:

- *Command Line*: The line into which you enter commands. If your command generates a result in the form of text, the result appears in the command line after the command executes: if there is no result, the box is empty after the command executes. In either case, the cursor reappears after execution, to show that the Spectrum RXI is again at Ready For Next Command.
- *Previous Command Line*: This is the last line of the scroll buffer, and it typically displays the previous command you executed. This repeat of the previous command is called a *command echo*.
- *Prompt Line*: This line displays information. In Figure 1-13, for example, the message reports that the Spectrum RXI will place the next scan in the Backg spectrum region.

- *Scan Status Box*: This box is always on the screen. It shows whether a scan is in progress, or whether the Spectrum RXI is ready to scan (as in Figure 1-13). When the external beam is selected for either the microscope or external bench accessory, the word **scan** above the scan status box changes to **external**.
- *Soft Key Labels*: The bottom line of the screen contains the labels for the seven soft keys. Only the soft keys that are available are displayed; in Figure 1-13, only four soft keys are displayed. If the label is highlighted, like the **BACKG** key in Figure 1-13, the command is executed immediately when you press the key; this is called an *action key.*

Entering a command

When you press a key that begins a command dialog, such as **scan**, the format of the user interaction area changes so that you can enter information.

Figure 1-14 shows the user interaction for the Scan command. Notice the following features:

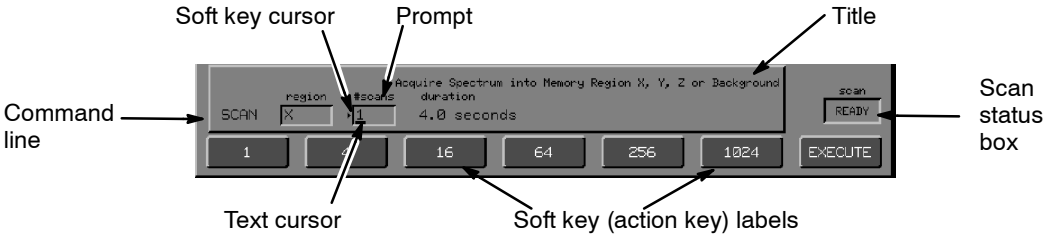


Figure 1-14 Command Line and Soft Keys for the Scan Command

- *Command Line*: The name of the command you are entering appears at the beginning of the command line. The box around the entire command line has disappeared; instead, each field where you can enter information is boxed separately. The boxes usually contain default entries, which you can change. (An unboxed field, such as **duration** in Figure 1-14, requires no entry; it provides you with information.)
- *Cursor(s)*: Either or both of two cursors may appear in the command line during a user interaction. Both appear at the **#scans** field in Figure 1-14. *The soft key cursor, an arrowhead just to the left of a field, identifies the active field when there is more than one interactive field, and indicates that you can use a soft key to make, or change, an entry in that field.*

The text cursor, a rectangle or flashing underscore within a field, indicates that you can use the keypad to type entries. You usually need to press **enter** *to accept typed entries.*

- *Title*: A title that reports the function of the command appears above and to the right of the command line.
- *Prompts*: Above each field is a prompt that defines the field.
- *Soft Key Labels*: The soft key labels in the bottom line show possible entries for the field to which the soft key cursor points. In Figure 1-14, all the keys are action keys.
- *Scan Status Box*: The scan status box is still displayed.

Executing a command

After you execute the Scan command, usually by pressing EXECUTE, the screen changes to Figure 1-15:

- All boxes and cursors disappear from the command line, so you can make no more entries.
- In some commands, new soft keys appear that you can use during command execution. For example, in Figure 1-15 detach and STOP are available.
- If the command initiated a scan, the scan status box no longer reports **READY**, but instead counts down as each scan is completed.

When execution of the command is complete, Ready For Next Command returns, with an echo of the command in the previous command line. If there is a result, it is reported in the command line.

Figure 1-15 Screen during Execution of the Scan Command

On-screen Help

You can display the on-screen help when the Spectrum RXI is at Ready For Next Command, or when you are within a command.

At Ready For Next Command

Two types of help are available:

- *help* – for example, a glossary, and the format of each typed command.
- *error help* – provides information on the previous error.

Within a command

Pressing **help** displays information about that command.

Entering Commands

There are four ways to enter commands with the Spectrum RXI:

- keypad keys;
- action keys;
- reverse entry;
- typed entries.

Keypad Keys

You usually enter commands with the labelled keys on the Spectrum RXI keypad. These keys are divided into groups according to their functions. The groups are illustrated in Figure 1-16 and described in the following table.

Group	Function
Task Keys	Collect spectral data. Change the screen display between graphics and text. Send output to the printer and plotter.
View Keys	Manipulate graphics displays on the screen.
Process Keys	Initiate various data-processing operations on spectra.
Calculator	Function as a spectroscopic calculator. Also used to enter numeric parameters in command fields.
Program Control Keys	Accept entries, cancel commands, restore previous system conditions.
Soft Keys	The soft key functions change as you access different command routines. Instead of permanent labels, soft keys have programmed labels on the screen.

Table 1-1 Groups of Keys on the Spectrum RXI Keypad

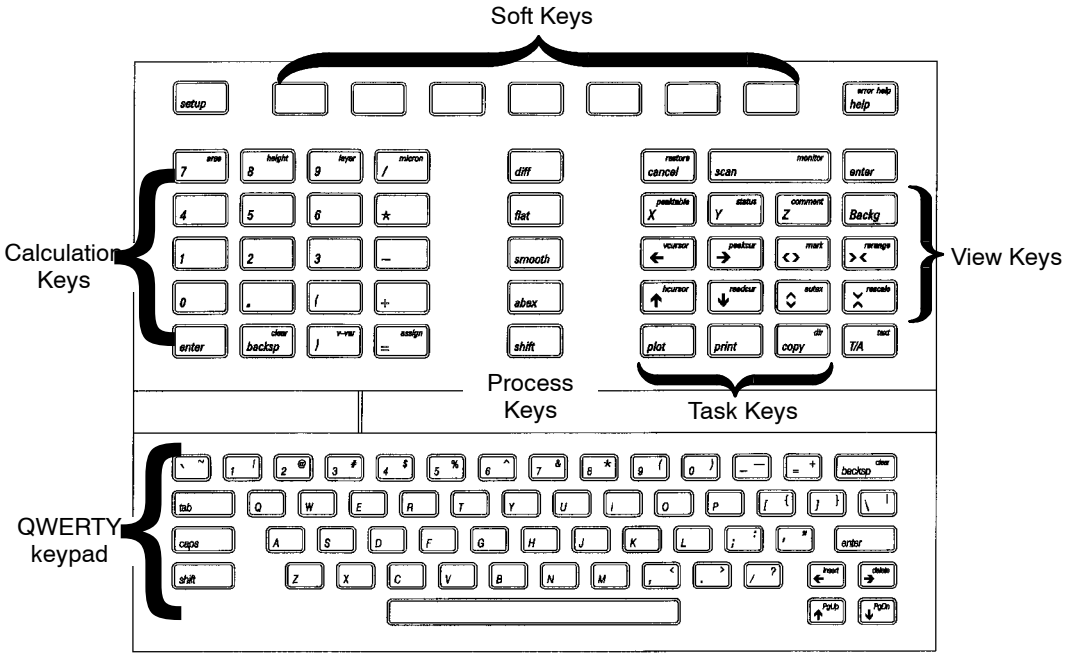


Figure 1-16 The Spectrum RXI Keypad

Keys that act immediately

Some function keys produce an immediate action. This may be because there is only one possible action for the key (for example, ***T/A*** or ***vcursor***), or it may be because it acts according to parameters set in Setup (for example, ***print*** and ***rerange***).

Keys that display a user interaction

Some keys access commands that require more information from you before they can be executed. For those commands, a user interaction screen appears.

To enter a command that has a user interaction:

1 Press the key that starts the command.
*The boxed fields of the user interaction appear on the command line. Figure 1-17 shows the user interaction for the Scan command. Above the command line, the title line gives the function of the command (***Acquire Spectrum...***).*

A soft key cursor (triangular), a text cursor (underscore), or both indicate the active field awaiting an entry. Both cursors are at the ***#scans*** *field in Figure 1-17.*

Figure 1-17 Entering Fields in a Command Line

2 Make the required entries in the command fields.
soft key entries*: If there is a soft key cursor just to the left of the field, press a soft key to make an entry in the field. If there is already an entry, pressing a soft key changes it.*

typed entries*: If there is a text cursor at the beginning of a field, type an entry into the field. Press* **enter** *when the field is correct.*

The cursor(s) may move to another field when you complete an entry. New soft keys may appear for entering the next field.

3 When all fields are correct, press **EXECUTE** .
The Spectrum RXI executes the command. An echo of the command moves into the previous command line, and any alphanumeric results are displayed in the command line.

When the cursor reappears at the beginning of the Command line, the Spectrum RXI is again Ready For Next Command.

NOTE: *As soon as* **EXECUTE** *appears, you can execute the command; a default value is used in any field where you have not entered a value.*

Action Keys

Action keys are soft keys that are highlighted. When you press an action key, the Spectrum RXI executes the command immediately; you do not have to enter any more information or confirm the operation.

- An action key may be the only key involved in a command, such as **Survey** at Ready For Next Command.
- Or an action key may be part of a user interaction. In that case, it provides one way to execute the command. The soft keys of the Scan user interaction in Figure 1-17 are all action keys.

Reverse Entry

Some commands that have user interactions can also be entered directly from the keypad, without using the soft key command routines. This is called *reverse entry*. To do this:

1 Type the numeric portion of the command.

2 Press the key that names the command.

Reverse entry can be used with **scan**, the three graphics cursors, and the arrow keys.

For example, to use reverse entry to collect 16 scans into the default spectrum region:

1 Type **16** with the number pad.

2 Press **scan**.

To use reverse entry to move the vertical cursor to 2225 cm^{-1}:

1 Type **2225** with the number pad.

2 Press **vcursor**.

Typed Entries

When the text cursor is displayed, you can type directly into the command line, using one of the following:

- the keypad of the Spectrum RXI;
- an auxiliary alphanumeric keyboard plugged into the **IBM KEYBD** connector;
- a terminal or computer connected to the **Remote PC** port.

You can type entries into fields of a user interaction, or you can type entire commands at Ready For Next Command.

Each command for the Spectrum RXI has a typed format. These are listed in Chapter 5 of *Advanced Operations*. The command echoes, which appear in the previous command line after each command is executed, use these same formats.

Using the Keypad

Uppercase (capital) letters can be typed in two ways:

- Pressing [shift] and then [A] types **A**.

NOTE: *Although* [shift] *can be used in the same way as* [shift] *on a typewriter, you do not need to hold it down while you press the key that you want to* shift*; the Spectrum RXI remembers that you have pressed* [shift] *until after the next keypress (enabling convenient one-handed use of the keypad). The* remembered shift *is indicated, where possible, by a change of cursor shape from underline to full rectangle. To cancel a* remembered shift*, press* [shift] *again.*

- Pressing [caps] locks the typing into capital letters until you press [caps] again.

Pressing the spacebar inserts spaces into text strings as they are typed.

Pressing [backsp] deletes the character to the left of the text cursor, leaving a space.

Pressing [clear] deletes the entire contents of the field.

[enter] has the same function as [enter] on the spectroscopic keypad.

When you type text, it overwrites any text that is there already.

Arrow keys

You can move the text cursor and insert and delete characters using the arrow keys on the spectroscopic keypad:

NOTE: *The following information only applies to alphabetic entries; for numeric entries, only* [backsp] *and* [clear] *are available (see above).*

- [◄] and [►] move the text cursor to the left and right within the text;
- [< >] and [insert] insert a space at the cursor position:
  Thesample [< >] **The sample**
  Thesample [insert] **The sample**
- [> <] and [delete] delete the character at the cursor position:
  The ssample [> <] **The sample**
  The ssample [delete] **The sample**

NOTE: [> <] *deletes the character at the cursor position;* [backsp] *deletes the character to the left of the cursor position.*

You can use the labelled keys on the spectroscopic keypad to type the names of commands or spectrum regions into comments. This feature is particularly useful when you are writing methods, and because of this, text that you type in this way is displayed in CAPITAL LETTERS.

When the field is full

Some alphanumeric fields (**comment**, for example) are longer than the space allotted for them on the screen. An open-ended box appears around these fields. When you fill the box with text, there is still more space in the field. As you continue adding characters, the text moves to the left.

When the entire field is full, you receive a warning: **Edit line full**. The warning disappears at the next keypress, and you can take action in any of the following ways:

- Ignore the warning. Each additional character you add to or insert in the string causes a character to be lost.
- Delete some characters before adding any more.
- Press [enter] to accept the line as it is, with no further additions or deletions.

Cancelling Tasks

The **cancel** key cancels the effects of previous commands; it functions differently depending on the situation:

- *During a user interaction* – before the command on the command line is executed, **cancel** stops the command with no echo to the scroll buffer and no result line. The Spectrum RXI returns to the state it was in before the user interaction began.
- *While a command is executing* – (during scan or monitor, for example), **cancel** stops the command with an echo of the cancelled command to the scroll buffer and a result line for the Cancel command. The Spectrum RXI returns to the state it was in before the cancelled command was issued, and saves no results of the command.
- *At Ready For Next Command* – pressing **cancel** enables you to cancel a detached task in progress. Tasks that can be performed in a detached mode are Scan, Plot, Print, and Format.
- *Deep in the Setup commands* – in deep levels of user interaction, typically in some of the more advanced Setup interactions, repeatedly pressing **cancel** returns you to Ready For Next Command.

NOTE: *If you press* **cancel** *at Ready For Next Command when there are no detached tasks in progress, the message* **Error: no detached tasks to cancel** *appears on the previous command line.*

Memory Locations

The Spectrum RXI provides memory locations for four different purposes, as shown in the following table:

Type of Location	Number Available	Designation	Function
Spectrum Regions	4	X, Y, Z, Backg	Store spectral data collected by the Spectrum RXI, ready for viewing and processing.
Store Regions	6	store1, . . . store6	Store spectral data for later recall into a spectrum region.
Method Regions	7	method1, . . . method7	Store lists of commands (methods) for later, repeated use.
Restore Region	1	Restore Region	Stores a copy of the last spectrum that was displaced from any spectrum region.

Table 1-2 Memory Locations in the Spectrum RXI

Spectrum Regions

The four spectrum regions (X, Y, Z and Backg) are the working memory regions that hold the spectra or interferograms collected with the Scan command. You can then view and process them as you require.

Spectra in the spectrum regions are lost when the Spectrum RXI is switched off, so save your data on disk before switching it off. If you do not have a disk drive, make plots of your important spectra.

The spectrum stored in Backg is used as the background when you scan in single-beam ratio mode. Under some circumstances, the Spectrum RXI prevents you from overwriting this region.

NOTE: *Although Backg is mainly intended to hold the background spectrum, the region may be used to hold any spectrum, in much the same way as X, Y and Z are used. However, when you copy data into the Backg region, the following message is displayed:* **Warning: current background will be overwritten***; subsequent scans may be ratioed against the modified background.*

Choosing a spectrum region to work on

When you enter a command, you usually use the *region keys* to choose the spectrum region whose data you want to process or the region where you want to place results. Some commands also provide soft keys for this purpose.

The default region

Each time you press a region key, that region becomes the *default region*. The Spectrum RXI assumes that you intend to continue using that region, and enters it in all **region** fields.

This means that after you have scanned into region Y, for example, you can continue to work with that spectrum without having to press [Y] again. Alternatively, whenever you want to view or process another spectrum, you need only press the appropriate region key.

Store Regions

The store regions provide temporary storage for spectra until you are ready to work with them. To store a spectrum in one of the store regions, use [copy].

Like the spectrum regions, the spectra in the store regions are lost when the Spectrum RXI is switched off.

Method Regions

A method is a list of commands that you store in one of the seven method regions. You can create methods using Method-Write, then execute them with the (method) soft key at Ready For Next Command.

Unlike the store regions, the method regions are not lost when you switch off the Spectrum RXI: they are in a non-volatile, battery-backed memory. You can also store methods on disk.

Instructions for storing and running methods are given in Chapter 6.

Restore Region

You will not usually be aware of the restore region. It provides a location where the Spectrum RXI can place a spectrum from a spectrum region when it would otherwise be overwritten.

If you want to restore the last spectrum you overwrote, use ***restore***; it usually enables you to transfer the spectrum from the restore region back into the region. See the Restore command description, starting on page 2-20, for a full explanation.

Setup: Setting User Preferences

When your Spectrum RXI is first installed, it is ready to run its first scan. All the operating parameters have been set by the factory at typical values. However, you can completely customize the Spectrum RXI for your particular needs by altering the operating parameters.

A wide variety of operating parameters is available:

- major experimental decisions, for example, scan range and operating mode (single-beam, ratio, or interferogram);
- features you may or may not choose to use, for example, including the user's name on files and plots;
- instrument features, for example, setting the system clock or adjusting the volume of the audible signal.

The *Spectrum RXI Tutorials* help you explore some of the available options. For a complete description of the setup options, see the appropriate chapter in this manual, or in *Advanced Operations.*

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Collecting a Background Spectrum

When Fourier Transform Infrared (FT-IR) spectrometers such as the Spectrum RXI record infrared spectra, the data they record is characteristic of both the sample and the spectrometer: the infrared source, detector, beamsplitter, and window material all contribute to the spectrum. Also, any infrared-active species in the optical path (in particular, atmospheric CO_2 and water vapor) add to the spectrum.

To remove the instrument and atmospheric characteristics, you must collect a background spectrum without a sample. The Spectrum RXI can then divide the sample spectrum by the background spectrum to calculate a ratio spectrum, which is largely independent of the characteristics of the spectrometer.

When there is no Background Spectrum

There is never a valid background scan (or anything else) in the Backg region at start-up, so **BACKG** is always present when you first switch on the power in ratio mode. The screen is similar to Figure 2-1.

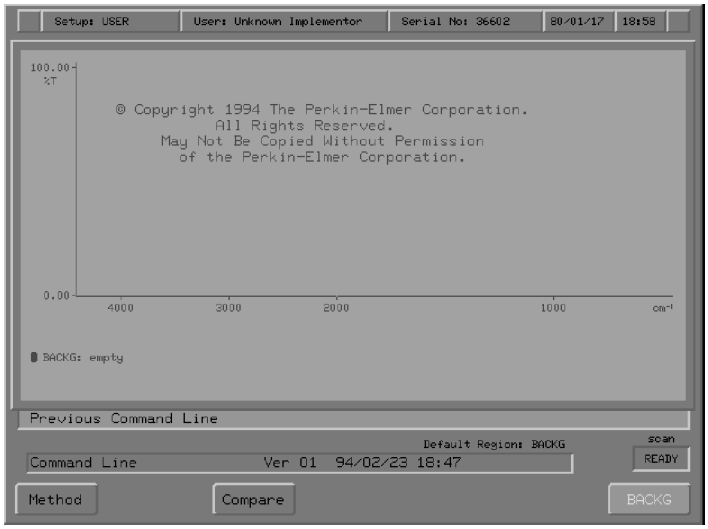


Figure 2-1 Screen at Start-up in Ratio Mode

NOTE: *If* BACKG *is available, you must collect a background. The destination spectrum region is Backg; you cannot change it.*

The action soft key BACKG collects one background scan and places it in the Backg spectrum region. BACKG is available if the following conditions are all true:

- the Spectrum RXI is at Ready For Next Command;
- the scan mode is **ratio**;
- there is no spectrum in the Backg spectrum region, or the spectrum in that region is not suitable for use as a background.

If the scan mode is not ratio or if there is a suitable background spectrum, the soft key is Survey. If a detached scan is in progress, the soft key is STOP, which stops the detached scan.

To be a valid background, the scan in the Backg region must:

- be a single-beam scan;
- have the same or higher resolution as is currently specified in Setup Scan options;
- include the scan range currently specified in Setup.

Collecting a single-scan background

1 Press **BACKG.**
The screen shown in Figure 2-2 is displayed.

- Empty axes are displayed, showing that new data are to be collected.
- The command line reports that the Spectrum RXI will collect one scan and place it in the Backg spectrum region.
- The status line reports that the scan is in single-beam mode.
- The only soft key is STOP. If you press this key, no data from the scan are saved, because one scan has not been completed. (See *Halting a Scan in Progress* on page 2-17.)

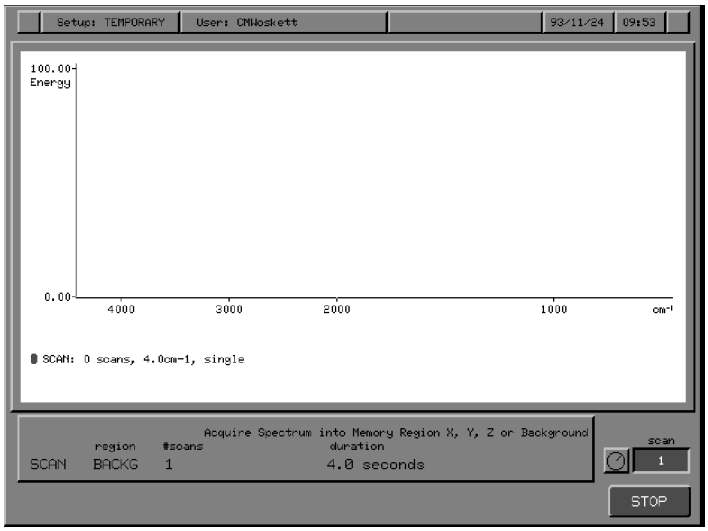


Figure 2-2 Collecting a Single-scan Background

When the scan is complete, Ready For Next Command returns (Figure 2-3).

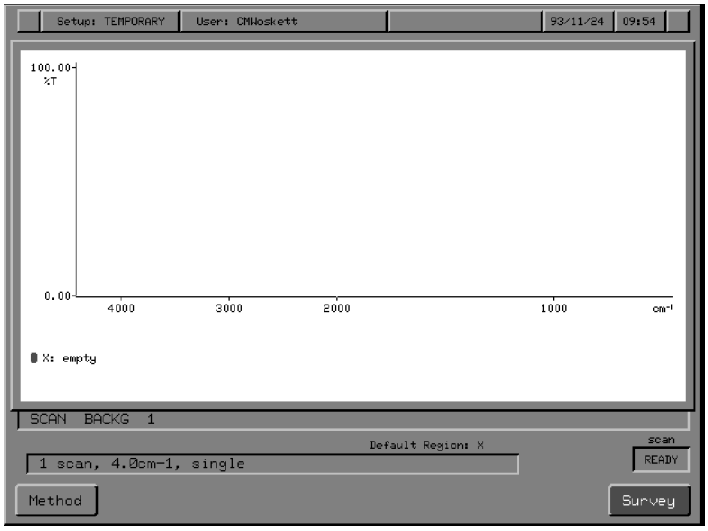


Figure 2-3 Ready For Next Command after a Background Scan

- Survey is now available instead of BACKG.
- The background spectrum is displayed in the axes for one second. Then X becomes the default region and is displayed.

NOTE: *You can also use the procedure described below to collect a background spectrum.*

When there is already a Background Spectrum

If there is already a suitable background in the Backg spectrum region (BACKG is not displayed at Ready For Next Command), you can still collect a new background spectrum.

When to collect a new background

You may need to collect a new background when:

- you want to work at a higher resolution;
- you need to collect a greater number of scans to improve the signal-to-noise ratio;
- the residual CO_2 and water-vapor bands in the sample spectrum increase to an unacceptable level;
- you change the sampling accessory.

NOTE: *During a day, the humidity and concentration of CO_2 and other infrared-active species in the air change, so you need to collect a new background spectrum frequently. Sometimes, for example when you use liquid cells with different window materials, you need to collect a new background for each spectrum.*

The following actions make the existing background incompatible. However, the Spectrum RXI recalculates the existing data to provide a new one for you the next time you scan:

- changing the scan range;
- changing to a lower resolution (for example, from 4 cm^{-1} to 8 cm^{-1}).

When you change to a higher resolution (for example, from 4 cm^{-1} to 2 cm^{-1}), the existing background spectrum becomes incompatible and the Spectrum RXI has no way to calculate a new one. In this case, BACKG replaces Survey at Ready For Next Command. If you press scan, the default destination region is Backg; you cannot enter a different destination until you have collected a compatible background spectrum.

Collecting a multiple-scan background

1 Press **scan**.
The screen in Figure 2-4 is displayed.

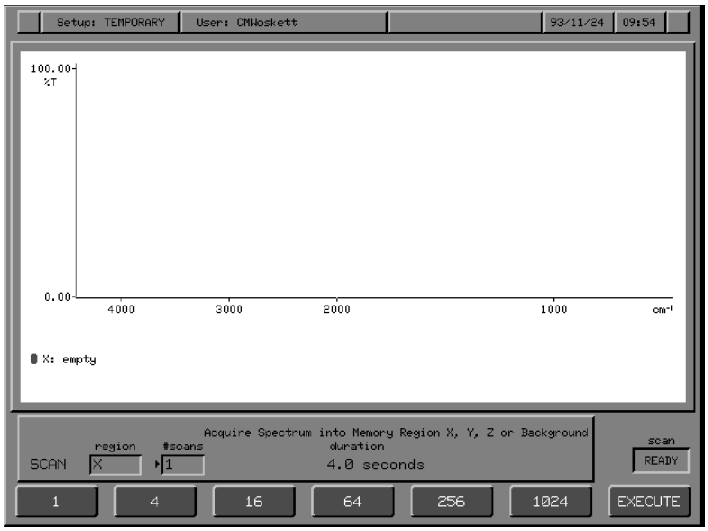


Figure 2-4 Initial Scan Screen

The default number of scans is the same number used for the previous Scan command. The current contents of the default region are displayed.

2 Press **Backg**.
The default region changes to **Backg**.

3 Choose the number of background scans you need: either type the number and press **EXECUTE**, or press the action key that corresponds to the required number of scans.
Scanning begins when you press an action key. The duration time for the number of scans is displayed.

Using the Backg Spectrum Region

The Spectrum RXI has four memory regions called spectrum regions, where you can place spectral data for display and manipulation. These regions are designated X, Y, Z, and Backg. You access them by pressing the corresponding keypad keys.

Using Backg in ratio mode

If the scan mode (set in the Scan Options of ***setup***) is ratio, the system divides the data from each new scan by the corresponding data in the background spectrum. The background spectrum is stored in the Backg (background) spectrum region. The Spectrum RXI will not collect a sample spectrum until there is a background spectrum.

Using Backg in other modes

When you are in single-beam mode or interferogram mode, the Spectrum RXI does not need a background spectrum. In these modes, you can use the Backg spectrum region interchangeably with X, Y, and Z to store interferograms or single-beam spectra. This gives you, in effect, four identical regions in which to view, process and plot spectra.

NOTE: *You can also copy data into Backg when you are using ratio mode, but when you next try to collect a ratio spectrum into one of the other spectrum regions, one of the following messages is displayed:* **Warning: background will be recalculated** *(if the scan setup is unchanged), or* **Warning: current background will be overwritten** *(if the scan setup is changed).*

Keeping the Backg Region Displayed

Usually, the last spectrum region used becomes the default region for the next operation. However, after a background scan, X is the default region because you do not usually scan another background immediately.

1. To keep Backg as the default region after background scans, type **set backg on** at Ready For Next Command.
2. To make X the default region after background scans, type **set backg off** at Ready For Next Command.

Collecting a Sample Spectrum

Collecting a Single Scan

Survey uses the scan mode currently established in Setup, and places one scan in the X region.

You can use survey scans as a quick way of:

- assessing the intensity of the spectrum, so that you can optimize the pathlength or concentration of your sample;
- assessing if the signal-to-noise ratio requires you to collect a multiple-scan spectrum.

1 Insert the sample in the sample compartment.

2 Press Survey.
The screen shown in Figure 2-5 is displayed.

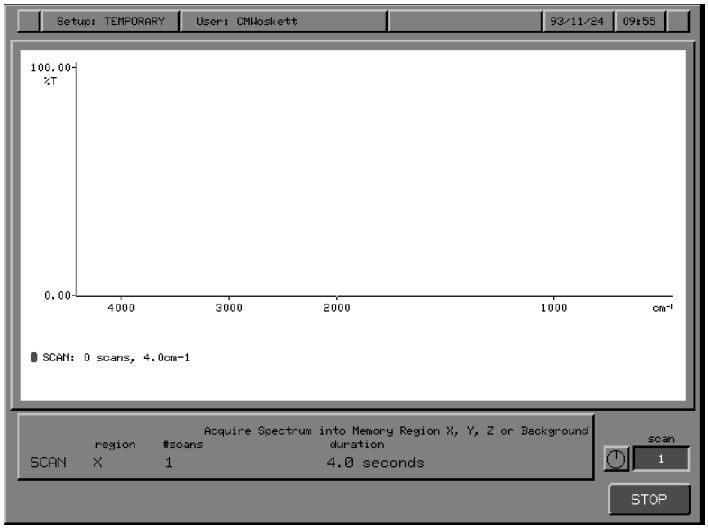


Figure 2-5 Collecting a Survey Scan

- Empty axes are displayed, showing that a new spectrum is being collected.
- The command line reports that the Spectrum RXI is collecting one scan and will place it in the default spectrum region.
- The only soft key is STOP. If you press this key, no data from the scan are saved, because one scan has not been completed.

When the scan is complete, the spectrum in the X region is displayed (Figure 2-6). Ready For Next Command returns.

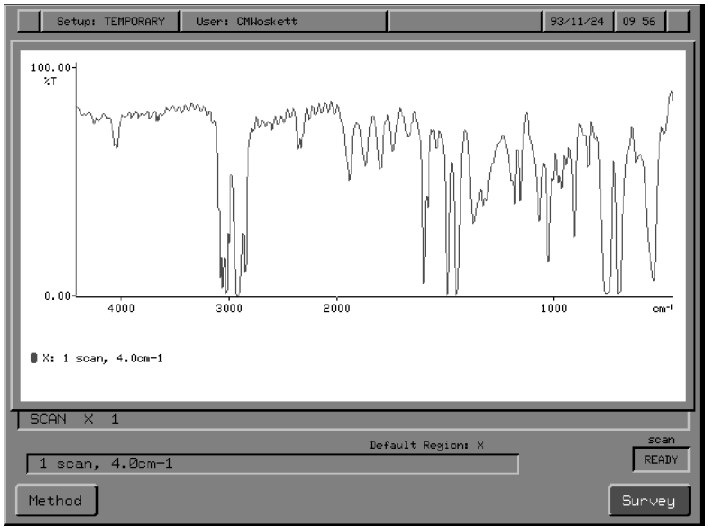


Figure 2-6 The Ready For Next Command Screen after a Survey Scan

Collecting Multiple Scans

Using the Scan command enables the Spectrum RXI to collect a specified number of scans, using the current settings of the Scan Options in Setup. The Scan Options are described in *Changing the Scan Options*, on page 2-22.

The data that are collected are placed in the spectrum region specified in the command.

Using Scan

1 If necessary, use the Scan Options in Setup to change the scan parameters. If you set the Scan Resolution to 2 cm^{-1} or 1 cm^{-1}, make sure that you insert the appropriate J-stop in the sample slide holder as described in *Inserting the Jacquinot Stop*, on page 2-40.

2 If the Spectrum RXI is in ratio mode and **BACKG** is displayed at Ready For Next Command, you must collect a valid background scan, as described in *Collecting a Background Spectrum*, on page 2-1.

3 Press **scan**.
The command line and soft keys shown in Figure 2-7 are displayed.

The default number of scans is the same number used for the last Scan command. The graphics display contains the current contents of the default region.

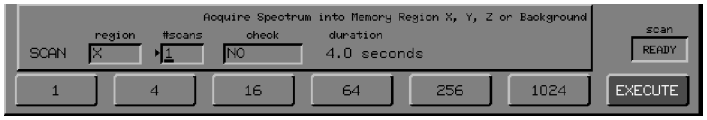


Figure 2-7 Initial Command Line and Soft Keys for the Scan Command

4 To change the spectrum region, press the appropriate region key.

5 Adjust the screen display with the arrow keys until the display represents the abscissa range and the ordinate scale you want to view during the scan.

NOTE: *The Scan Range option in Setup determines the range over which data are collected. The View Keys affect only the screen display. The View Keys remain active during the scan, so you can adjust the display at any time.*

6 Type the number of scans you require and begin the scan. Do this in one of the following ways:

- Press **scan** again.
  Pressing **scan** *a second time is equivalent to pressing* **EXECUTE**. *You can begin a scan by pressing* **scan** *twice in succession. This type of scan uses the default region and number of scans.*

- Type a number of scans, then press **enter**.
  The Spectrum RXI calculates a duration for the scan and displays it in the command line.

  If the duration is satisfactory, press **EXECUTE** to begin scanning. If the duration is not satisfactory, change the number of scans and press **enter**.

- Press one of the action keys to enter a number of scans.
  Scanning begins immediately. The duration for that number of scans is displayed.

When scanning begins, the display area clears briefly then the axes for the destination region are displayed. The action keys shown in the screen below become available. (If the duration is less than one minute, **detach** is not available.)

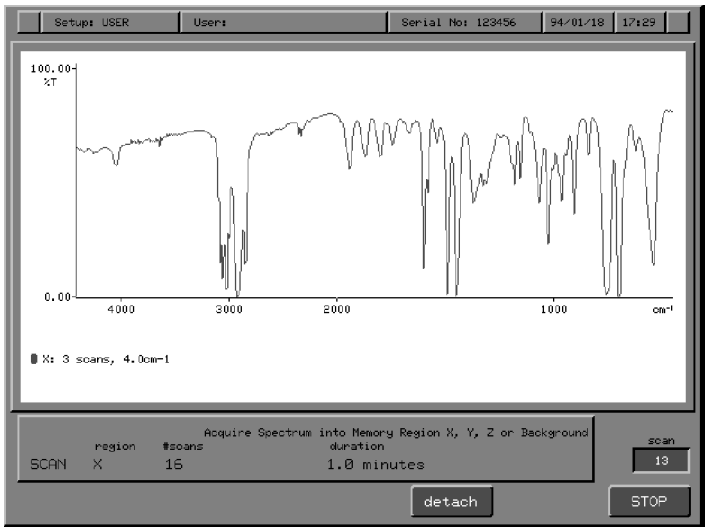


Figure 2-8 Screen During Execution of the Scan Command

- If you do not detach the Spectrum RXI from scanning (see *Multi-tasking using Detach* on page 2-13), the collected spectrum is displayed, and updated regularly.
- The scan status box counts down the number of scans still to be collected.
- The graphics status line under the spectrum reports the number of scans collected; it counts up as the scan status box counts down.
- As each scan is collected, the data from that scan are Fourier transformed and averaged with the data already collected.

The spectral data are collected into a special scan region of memory (Figure 2-9). When all the scans have been collected, the Spectrum RXI places the collected data in the spectrum region that was specified in the command. Or, if the scan has been detached, the data are held in the scan region until you attach the scan and designate a destination spectrum region.

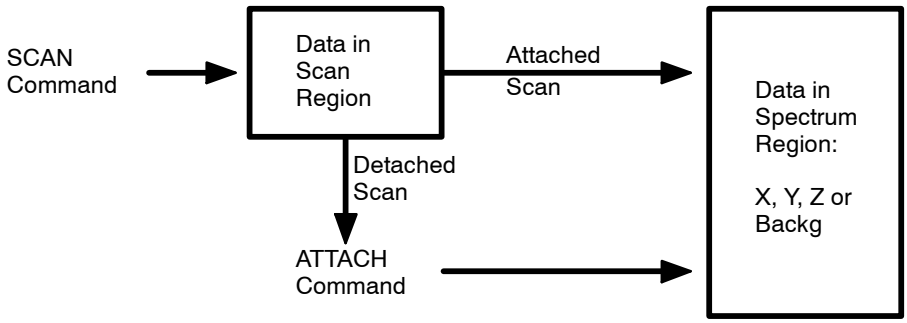


Figure 2-9 Storage of Scan Data from Attached and Detached Scans

Short Form of the Scan Command

You do not need to start the scanning using the prompted scan dialog; you can also use a short form:

Format	Example	Action
n **scan**	**16** **scan**	Collects **n** scans and places the resulting data in the default spectrum region.
region n **scan**	**X 16** **scan**	Collects **n** scans and places the resulting data in the specified spectrum region.
scan **scan**		Repeats the last scan: the scan type, number of scans, and spectrum region are the same.

Multi-tasking using Detach

The Spectrum RXI has true multi-tasking capabilities: you can use the Spectrum RXI to work with spectra that you have collected previously while it is collecting another spectrum. The scan data that are being collected are held in the scan region, and not placed in a spectrum region, so you can use the original destination region.

If the scan duration is more than one minute, ***detach*** is available during the scan. If you press this key, Ready For Next Command returns.

While the scan is detached, ***attach*** is available (Figure 2-10). When you press ***attach***, soft keys are displayed that enable you to select a new spectrum region as the destination for the scan.

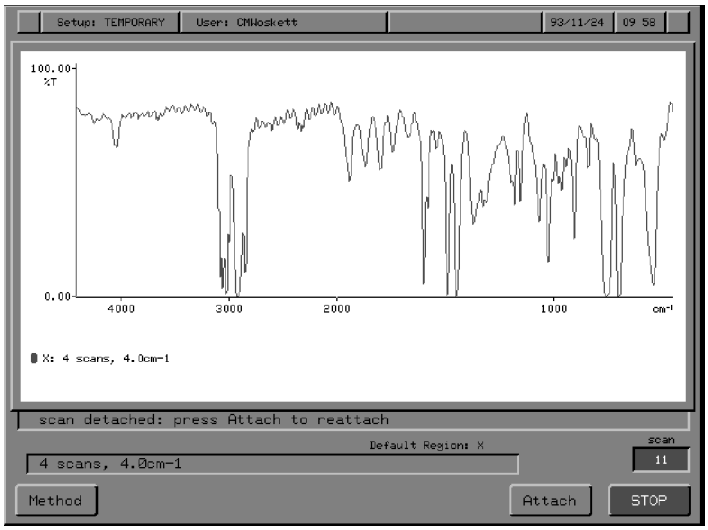


Figure 2-10 Re-attaching a Scan

When a detached scan is running in ratio mode, the Spectrum RXI protects the background scan by preventing you from issuing any command that would overwrite the Backg region. At other times, you can overwrite the background.

Scanning for a Specified Length of Time

When you enter a number of scans in the Scan command line, the Spectrum RXI calculates and reports a corresponding scan duration. This is the total time it will take the Spectrum RXI to collect the indicated number of scans, excluding the time for the final Fourier transform.

To scan for a certain amount of time:

1 Type an estimated number of scans in the **scans** field.

2 Press ***enter***.

3 Note the time that is reported in the **duration** field.

4 Modify the number of scans, if necessary, and repeat the process to make the duration what you require.

Interpreting the Scan Status Box

The scan status box is always displayed, above the right-hand soft key label. It tells you whether the Spectrum RXI is available for collecting data. Table 2-1 explains the various messages that are displayed in the scan status box.

Message	Condition	Explanation
READY	No scan in progress	OK to begin a scan.
# scans remaining	Scan in progress	The status box counts down as the scans are completed.
REJECT		The data in the current scan have been rejected. Countdown resumes with the next valid scan. The number of rejected scans is reported when you press **setup others others test scan history**.
PAUSE		The external scan enable line at the INPUT port is disabled. Scanning continues, but no data are collected.
OVRLOAD		The gain is too high.
FAIL		A fatal error has occurred. The scan terminates, and data collected prior to the error are kept. An error message is displayed on the result line.
STOP	A scan was stopped	The Spectrum RXI is completing the current scan. The status box then displays **COMPUTE**.
WAITING	Scan held	The Spectrum RXI is waiting for the scan hold input line to be released.
ENDING		The scan is returning to its resting position.
ERROR		A severe scan disturbance has occurred, and the scan action must be restarted.

Table 2-1 The Scan Status Box (continues overleaf)

Message	Condition	Explanation
COMPUTE	The final scan is complete	The data from the final scan are being Fourier transformed. When the transform is complete, the status box displays **DONE** for a detached scan, or **READY** for an attached scan.
DONE	Detached scans complete and transformed	The status box continues to display **DONE** until you attach the scan. If, instead, you start another scan, the detached scan data are lost.

Table 2-1 (continued) The Scan Status Box

Halting a Scan in Progress

To halt a scan in progress, you have the choice of using STOP or cancel. If you press either of these keys before the data from the first scan are displayed, the scan halts as if you had never issued the Scan command. If the screen is displaying spectral data from the scan, the two keys have different effects:

- When you use STOP, the data collected so far are kept.
- When you use cancel to halt the scan, all data collected are lost, and the previous contents of the destination region are restored.

The following table summarizes the action of each key with both attached and detached scans.

Status of the Present Scan	Action of STOP	Action of cancel
attached	Scanning stops. Data displayed on the screen are transferred to the default region.	Scanning stops. The default region is restored to its previous condition.
detached	The present scan is completed and its data transformed. The scan status is **COMPUTE** during the transform, then **DONE** until the data are attached.	Soft keys display the detached tasks that you can cancel. If you execute a new scan, the data are lost.

Table 2-2 Action of STOP and cancel with Attached and Detached Scans

Adding More Scans to a Spectrum

You can add more scans to the data from the previous Scan command by pressing [+] and typing a number in the **#scans** field of the Scan command line.

NOTE: *You can only continue adding scans to the spectrum collected immediately before. If the spectrum you collected previously was in X, and you continue scanning in Y, then the Spectrum RXI adds scans to the spectrum that is in X, but stores the resulting spectrum in Y. This gives you the original spectrum in X and the new spectrum with more scans in Y.*

For example, suppose that the previous Scan command collected 16 scans. To add data from four more scans:

1 Press [scan].

2 Type **+4**.
4 *is displayed in the* **#scans** *field.*

3 Press EXECUTE.
Data for 20 scans are sent to the default region.

An error message is displayed if you try to continue a scan in the following situations:

- after changing the resolution;
- if you try to continue a cancelled scan;
- if you have used [monitor] since the previous scan.

NOTE: *When you STOP a scan, the Spectrum RXI memory contains approximately three more scans than have been transformed and displayed. If you then continue the scan, the additional scans are added to all the data in memory.*

Recalculating a Spectrum

The Spectrum RXI can recalculate the previous spectrum using a different apodization, resolution, or range, provided you have neither used **monitor** since the last scan, nor changed to a higher resolution (for example, from 4 cm^{-1} to 2 cm^{-1}).

1 Change the apodization, resolution, or range in the Scan Options (see page 2-22 onwards).

2 Press **scan**.

3 Type **+0**.

4 Press **EXECUTE**.
The recalculated data are stored in the default region.

Restoring a Spectrum to a Region

Each time you use a command that places a spectrum in a spectrum region, the spectrum that was previously there is moved to the restore region. By pressing ***restore***, you can return that previous spectrum to the spectrum region.

Figure 2-11 shows how the software uses the restore region of memory:

A Suppose a spectrum called SPEC1 is in spectrum region X, and a displaced spectrum SPEC0 is in the restore region.

B If you begin the Scan user interaction, but cancel before executing the command, SPEC1 is still in X, and SPEC0 still in the restore region.

C However, if you execute the scan, a new spectrum SPEC2 is collected into region X, and SPEC1 displaces SPEC0 in the restore region

D If you use ***restore*** to restore the spectrum in X, SPEC1 returns to region X, SPEC2 goes into the restore region, and SPEC0 will never return.

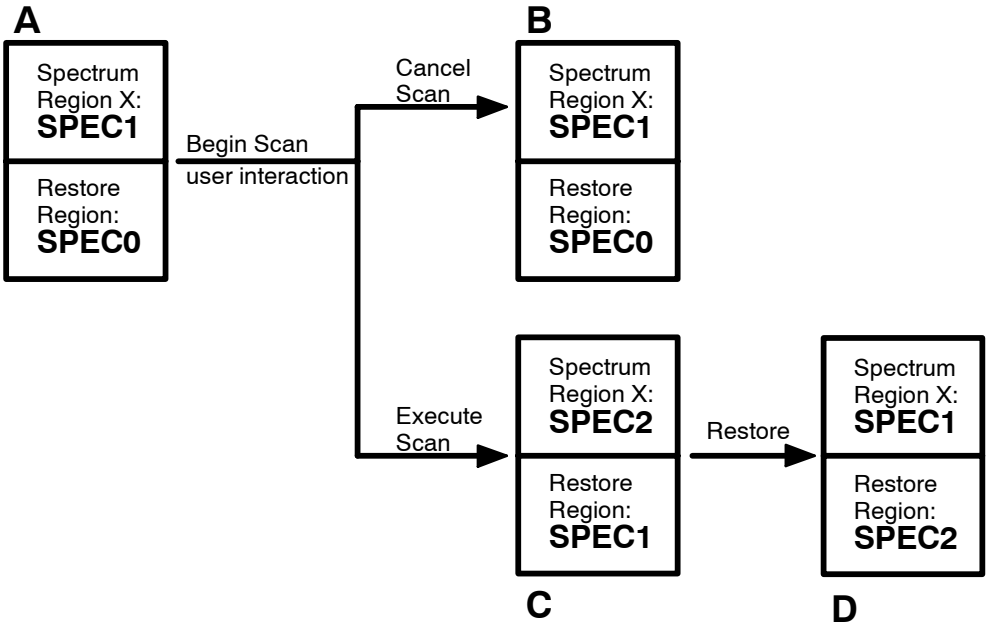


Figure 2-11 Restoring a Spectrum to a Region

Using the Restore Command

1 Press **restore**.
The Restore command line appears. (An example is shown in Figure 2-12). Soft keys are present for the Restore functions that are currently valid: in addition to restoring a spectrum to a spectrum region, you can also restore a setup and unlock the keypad.

NOTE: *If a region soft key does not appear in the left-most soft key position, you cannot restore a spectrum.*

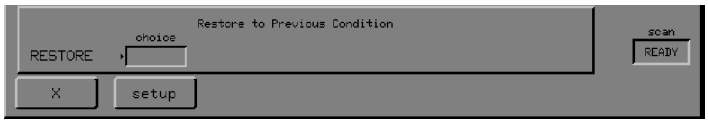


Figure 2-12 The Restore Command Line and Soft Keys.
(You can restore a spectrum to region X, and a setup.)

2 Press the region soft key.
The contents of the restore region are displayed.

3 To restore the spectrum, press **EXECUTE**.
The spectrum is restored to the region from which it came.

or

Press **cancel**.
Ready For Next Command returns.

Changing the Scan Options

The Scan options affect how the Spectrum RXI collects spectra.

Accessing the scan options

1 At Ready For Next Command, press **setup** **scan** .
The table and soft keys shown in Figure 2-13 are displayed. Figure 2-13 shows the factory default values for the Scan options. If the scan mode is **igram***, the table does not include resolution and apodization. If your Spectrum RXI does not have an accessory with an external detector, the table does not include* **gain** *or* **speed.**

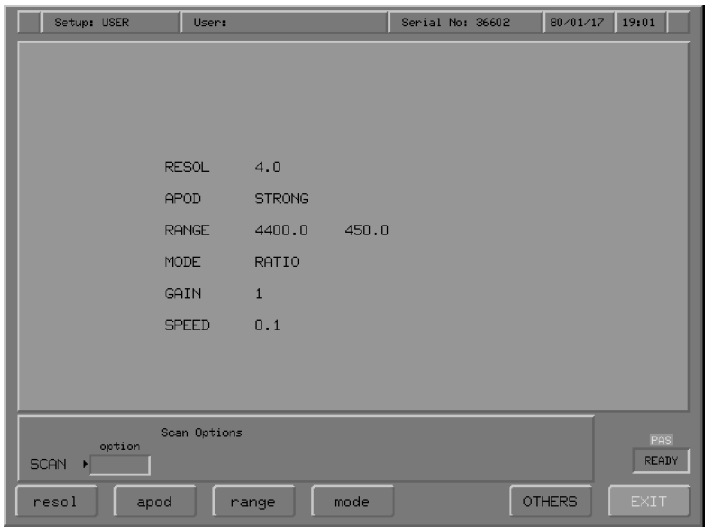


Figure 2-13 The Scan Options Screen

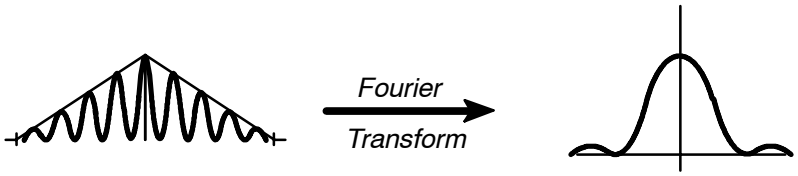
The following pages define the various Scan options and explain the choices available for each.

Apod(ization)

An FT-IR spectrometer generates an interferogram by scanning a moving mirror over a finite distance. However, to ensure that all information is collected, the interferogram needs to extend between plus and minus infinity. By stopping the mirror, we truncate the interferogram and limit the resolution; it is as if the interferogram had been multiplied by a *boxcar* function:

Notice that this boxcar truncation introduces lobes, or *feet*, at the sides of the peak. These feet are a result of the abrupt end of the data collection.

Apodization is the mathematical process used to remove these feet (apodization is from the Greek *αποδ - apod*, meaning *without feet*). One way of removing these feet is to use a triangular apodization, which gives less weight to the data at the ends of the interferogram:



Notice that, although the feet are smaller, the peak is broader. When a spectrum is apodized, the full width at half height (FWHH) of the peak can be up to twice as large as the FWHH of the unapodized peak.

There are many different, elaborate apodization functions, which try to find the best compromise between removing the feet and limiting the peak-broadening. The Spectrum RXI gives you the option of selecting from the most widely used. The Scan Apod option gives you a choice of weak or strong Beer-Norton apodization, or no apodization at all, that is, Boxcar. Figure 2-14 shows the effect of both weak and strong Beer-Norton apodization, compared to a band with no apodization. Notice that the strong Beer-Norton apodization eliminates the artifacts completely in this case, but broadens the band more than does the weak Beer-Norton.

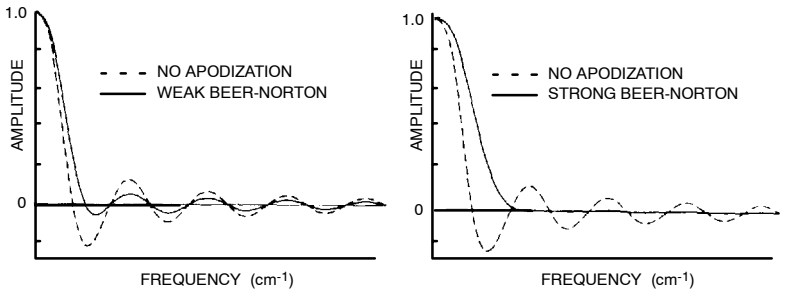


Figure 2-14 Weak and Strong Beer-Norton Apodization Compared to a Band with No Apodization

Advice on choosing an apodization function

For most applications, the strong Beer-Norton apodization function is the most appropriate. For gas-phase samples, you can get a higher resolution by using a weak Beer-Norton, but you need to make sure that the spectrum has strong absorption lines, to avoid losing spectrum detail in the ripples.

Setting the apodization function

1 At Ready For Next Command, press **setup** **scan** **apod** .
The command line and soft keys in Figure 2-15 are displayed.

Figure 2-15 The Scan Apod Command Line and Soft Keys

2 Choose the apodization function you require or, to execute the current command line without changing the apodization, press **EXECUTE** .
The Scan Options screen returns.

Gain

The Scan Gain option is available only if a PAS (photoacoustic detector) is fitted. It enables you to change the gain of the external preamplifier.

- If the scan status box reports **OVRLOAD** during a scan, you need to reduce the gain.

Setting the gain

1 At Ready For Next Command, press **setup** **scan** **gain** .
The command line and soft keys in Figure 2-16 are displayed. The numbers on the soft keys represent factors by which you can multiply the gain. The range of gain values is from 1 through 128. To display the soft keys for the higher scan speeds (Figure 2-17), press **OTHERS** .

Figure 2-16 The First Scan Gain Command Line and Soft Keys

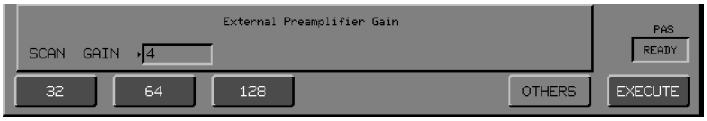


Figure 2-17 The Second Scan Gain Command Line and Soft Keys

2 Choose the gain factor you require.
The Scan Options screen returns. The displayed table shows the changed setting of Scan Gain.

Mode

The Scan Mode Option gives you a choice of three scan modes:

Mode	Description
ratio	single-beam ratio. The data are ratioed to a background spectrum that is in the Backg spectrum region.
single	single-beam. The spectrum is not ratioed.
igram	processed interferogram. The spectrum is processed to remove offsets, and displayed on a μm abscissa scale.

Table 2-3 Scan Modes in the Spectrum RXI

Selecting a scan mode

1 At Ready For Next Command, press **setup** **scan** **mode** .
The command line and soft keys in Figure 2-18 are displayed.

Figure 2-18 Scan Mode Command Line and Soft Keys

2 Choose the mode you require or, to keep the current scan mode, press **EXECUTE** .
The Scan options screen returns.

Range

The scan range is the range over which the Scan command collects data. The scan range set as the default at the factory is 4400 to 450 cm^{-1}. The scan range is also the default range to which ***rerange*** sets the screen display. If you change the scan range, the Spectrum RXI also changes the View Rerange limits to the same values.

You can set the scan range to whatever you require, within the following limits:

total length	at 1 cm^{-1} resolution, 4000 cm^{-1}; at lower than 1 cm^{-1} resolution, up to the entire range of the instrument (7800 to 100 cm^{-1}).
upper limit	7800 cm^{-1}.
lower limit	100 cm^{-1}.

In igram mode, the scan range is -10 000 to 2000 μm.

Changing the scan range (and View Rerange limits)

1 At Ready For Next Command, press ***setup*** (***scan***) (***range***).
The command line and soft keys shown in Figure 2-19 are displayed. The alphanumeric cursor is in the **from** *field.*

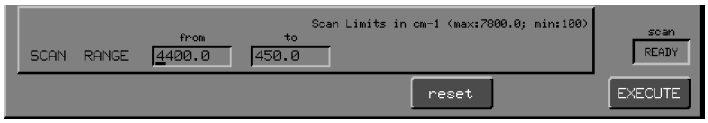


Figure 2-19 Scan Range Command Line and Soft Keys

2 If you want to reset the scan range to the default limits set at the factory, press ***reset***.
The Scan options screen returns.

3 If you want to change the upper limit of the scan range, type a number. If not, go to step 4.

4 Press ***enter***.
The alphanumeric cursor moves to the **to** *field.*

5 To change the lower limit, type a number.

6 Press ***EXECUTE***.
The Scan Options screen returns.

Resol(ution)

An FT-IR spectrometer collects a spectrum by scanning a moving mirror to produce an optical path difference (OPD) between two arms of an interferometer. This creates an interference pattern called an interferogram, which can be converted into a spectrum by a mathematical process called Fourier transformation.

The farther the moving mirror scans, the higher the resolution of the spectrum is. That is, the longer the interferogram, the more fine structure is resolved in the spectrum.

Resolution is inversely proportional to the mirror displacement: high resolution, corresponding to long interferograms, is therefore represented by a small numerical value. 1 cm^{-1} is said to be a higher resolution than 4 cm^{-1}.

The Jacquinot stop

When the moving mirror scans, off-axis rays from the infrared source degrade the theoretical resolution described above. You can keep the effective resolution close to the theoretical value by placing a circular aperture called the Jacquinot stop (J-stop) in the beam. This limits the amount of off-axis rays that reach the detector. The size of the J-stop needed to do this depends on how far the moving mirror scans.

High resolution spectra need a small J-stop aperture to keep the effective resolution close to the theoretical value. The size of the J-stop also depends on the wavenumber of the peak you are interested in: to achieve a resolution of 1 cm^{-1} at 4000 cm^{-1}, you need to use a smaller J-stop aperture than to achieve the same resolution at 2000 cm^{-1} .

To insert the J-stop into the sample-slide, follow the procedure on page 2-40.

Advice on choosing a suitable resolution

Infrared spectra of solid and liquid samples have broad absorption bands that are usually at least 10 cm^{-1} wide. For these samples, 4 cm^{-1} usually resolves all the fine structure and often 8 cm^{-1} is adequate. By using the lowest adequate resolution (for example, 8 cm^{-1} rather than 4 cm^{-1}), you reduce the data collection time and improve the signal-to-noise ratio.

For samples of gases you almost always need to use the highest resolution available. The infrared absorption bands of gases show sharp rotational fine structure that is characteristic of the structure of the molecule.

Increasing throughput

When you use the Spectrum RXI at resolutions of 1 and 2 cm^{-1}, you need to insert a J-stop into the sample slide (refer to page 2-40) if you are interested in bands above 2000 cm^{-1}. If you are only interested in bands between 2000 and 400 cm^{-1}, you need not use a J-stop; this does not degrade the resolution and maintains a high throughput, and therefore a good signal-to-noise ratio.

With the appropriate J-stop inserted, 1 or 2 cm^{-1} resolution is maintained up to 7800 cm^{-1}.

NOTE: *If you want to use 1 cm^{-1} resolution but this soft key is not displayed, reduce the scan range (see page 2-27).*

Setting the resolution

1 At Ready For Next Command, press **setup** **scan** **resol** .
The command line and soft keys in Figure 2-20 are displayed.

Figure 2-20 Scan Resol Command Line and Soft Keys

2 Choose the required resolution, or type the resolution you require and press **EXECUTE** . (You can type a resolution in the range 64 cm^{-1} to 1 cm^{-1}; decimal values are allowed.)
The Scan Options screen returns.

3 If you set the resolution to 1 or 2 cm^{-1}, make sure that you insert the appropriate J-stop in the sample slide.

Speed (OPD Velocity)

The Scan Speed option is available only if a PAS (photoacoustic detector) is fitted.

OPD velocity The OPD (optical path difference) is the difference in optical path between the two beams of the interferometer. The OPD velocity, or scan speed, for an interferogram is the rate at which the OPD is varied.

NOTE: *The Spectrum RXI automatically selects the best scan speed for the currently-selected detector (0.3 cm/s for the $LiTaO_3$ detector supplied). However, for the optional PAS, the effective penetration depth of light into the sample is a function of scan speed. Because you can choose the scan speed for PAS, you can collect more information about some samples.*

Setting the scan speed

1 At Ready For Next Command, press **setup** (scan) (speed).
The command line and soft keys in Figure 2-21 are displayed. The numbers on the soft keys represent the scan speeds that you can choose.

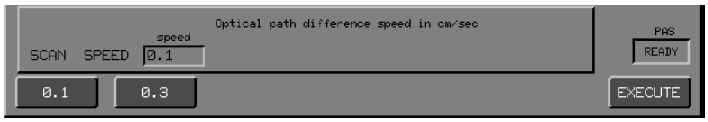


Figure 2-21 The Scan Speed Command Line and Soft Keys

2 Choose the scan speed you require.
The Scan Options screen returns. The displayed table shows the changed setting of Scan Speed.

Monitoring the Current Signal

monitor enables you to observe various signals while the Spectrum RXI is scanning. Monitoring is useful when you are aligning the interferometer, setting up an accessory, or determining the progress of purging.

Signals you can Monitor

The signals available for monitoring vary depending on the scan mode. The following table reports what you can monitor in each mode.

Scan Mode	Signals Available
Single-beam	energy throughput, raw interferogram, single-beam scan
Ratio	energy throughput, raw interferogram, ratio scan, background
Interferogram	energy throughput, raw interferogram, scan (processed interferogram – the interferogram is filtered, scaled and interpolated to a μm abscissa scale)

Table 2-4 Monitoring in Various Scan Modes

While you are monitoring one type of signal, the soft keys remain available to enable you to select one of the other types. You do not have to return to Ready For Next Command to change signals.

Whenever you use ***monitor***, the previous scan is overwritten in the internal memory of the Spectrum RXI. Because of this, you cannot continue a previous scan after using ***monitor***.

Using the Monitor Command

1 Press **monitor**.
The command line in Figure 2-22 is displayed.

Figure 2-22 Initial Command Line and Soft Keys for Monitor

2 Press the soft key that corresponds to the signal you want to monitor.
All the soft keys except **igram** *are action keys; when you press one of them, monitoring begins at once. The* **type** *field tells you the signal you are monitoring. The soft keys remain available so that you can change the type of signal.*

3 To change the type of signal being monitored, press another soft key.

4 When you want to stop monitoring, press **STOP**.
Ready For Next Command returns. The command echo **MONITOR** *is reported in the Previous Command line.*

Monitoring the Raw Interferogram

1 Press (igram).
The command line in Figure 2-23 is displayed.

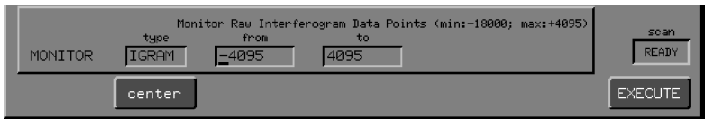


Figure 2-23 The Monitor Igram Command Line

2 You must decide what range you want to monitor. The choices are:

To accept the default range: press EXECUTE.

or

To change the range of the interferogram you are monitoring:

a Type the lower limit of the range you want to monitor. (The command line tells you the allowed range.)

b Press enter.

c Type the upper limit of the range you want to monitor.

d Press EXECUTE.

Monitor only the centerburst

1 If you want to monitor only the centerburst, press center .
The display becomes similar to Figure 2-24.

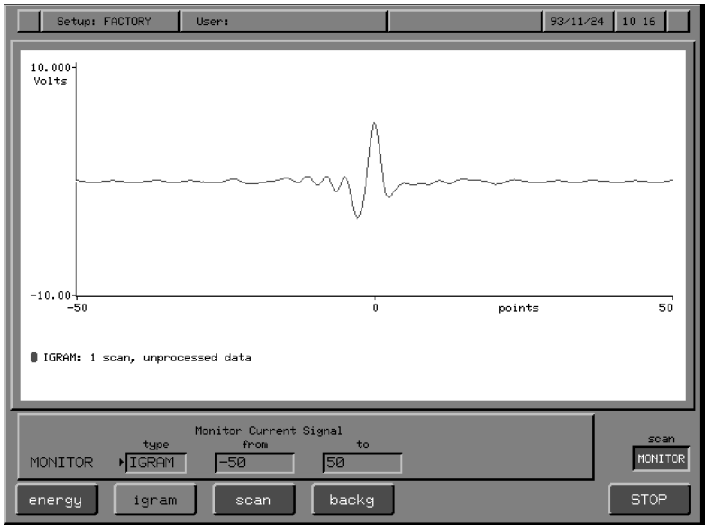


Figure 2-24 Monitoring the Centerburst

Whatever the range you selected to monitor, the command line now reports that range, the view range changes to coincide with the new scan range, and the soft keys become as they were at the start.

Monitoring the Energy Throughput

The graphics display for energy monitoring consists of a bar graph with a logarithmic scale, as shown in Figure 2-25. The greater the energy throughput, the longer the bar. As you adjust the Spectrum RXI, the greatest length the bar has attained is indicated. The number above the bar is in arbitrary units, which are related to the height of the interferogram.

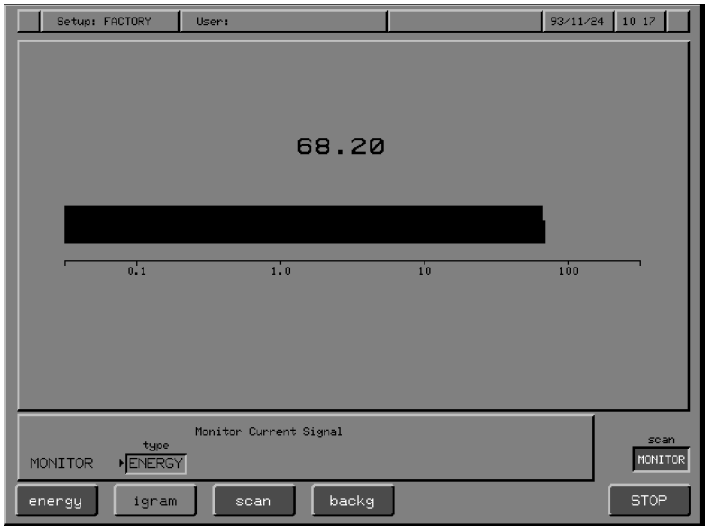


Figure 2-25 Monitoring the Energy Throughput

Monitoring the Scan

Monitoring the scan gives different output depending on the scan mode:

Scan Mode	Output of MONITOR SCAN
single	single-beam spectrum
ratio	the spectrum is ratioed to the existing background spectrum. If no background exists, scan is not available and the following message appears: **new background required.**
interferogram	processed interferogram over the scan range established by Setup.

Table 2-5 Effect of Scan Mode on Output of MONITOR SCAN

You can use the view keys to adjust the display scales. (Because Monitor does not display the spectra in the spectrum regions, the region keys are invalid.)

Monitoring the Background

The option of monitoring the background spectrum is only available in ratio mode. The background is a single-beam spectrum, similar to the one shown below.

NOTE: *When you use the Monitor Backg command, you are monitoring a single-beam spectrum, for example, the background spectrum; if there is a sample in the sample slide, you monitor the single-beam spectrum of that sample.*

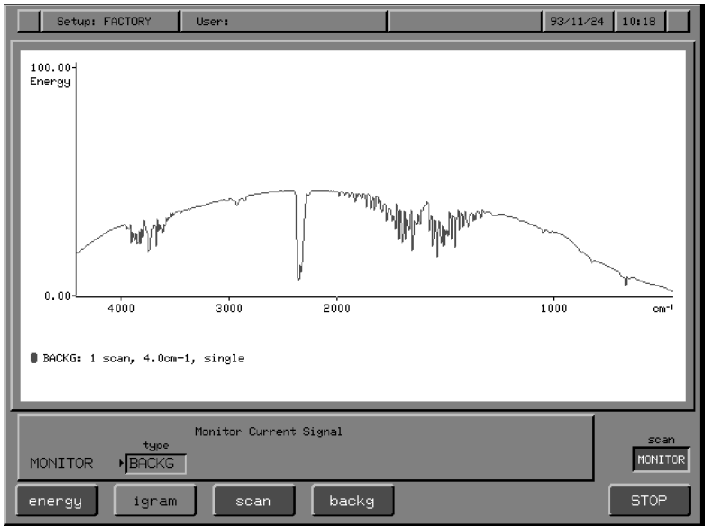


Figure 2-26 Monitoring the Background Spectrum

Using the Sample Compartment

J-stops

1 cm^{-1} and 2 cm^{-1} J-stops

When you use the Spectrum RXI at resolutions of 1 and 2 cm^{-1}, you need to insert a J-stop into the sample slide if you are interested in bands above 2000 cm^{-1}. If you are only interested in bands between 2000 and 400 cm^{-1}, you need not use a J-stop; this does not degrade the resolution and maintains a high throughput, and therefore a good signal-to-noise ratio. To identify the appropriate J-stop, the 1 cm^{-1} has one hole in the bent end, and the 2 cm^{-1} J-stop has two (see Figure 2-27).

Half-aperture stop

The *half-aperture* stop has a rectangular cut-out that enables only the top half of the beam to pass through. The stop is used to suppress back reflections from highly reflective samples, which might otherwise generate spurious features in the spectrum.

Typical applications where the stop may be useful include careful measurements of the transmission of interference filters and crystal plates.

When such samples are placed perpendicular to the beam, radiation reflected from the surfaces of the sample re-enters the interferometer, where it is modulated for a second time by the scan mechanism. If this doubly-modulated light then re-emerges from the interferometer to reach the detector, the spurious signal appears to the Fourier Transform to belong at twice its actual wavenumber. The result is apparent stray light at higher wavenumbers, especially above 4000 cm^{-1} where normally transmitted energy from the source starts to decrease.

The half-aperture stop works by preventing reflected light from re-emerging from the interferometer, at the expense of reducing the normal throughput by a factor of approximately two.

NOTE: *For typical measurements of organic samples in the region below 4000cm^{-1}, the stop is not needed because these reflective effects, although still present, are usually negligible in relation to the primary spectrum signal.*

Reference aperture

The *reference aperture* stop has a 10 mm circular aperture and is easily distinguished from the $2cm^{-1}$ stop by the absence of small holes punched in the bent end.

The stop is used to limit the beam diameter in some instances where otherwise the sample cell would clip the edges of the infrared beam.

A typical application of the stop is in the careful measurement of KBr disk samples using the sample shuttle. In this measurement, the background spectrum is recorded with the sample cell out of the beam. When the ratio spectrum is measured, the sample cell clips the edges of the beam, reducing the effective J-stop size slightly. This in turn changes the resolution slightly with the result that sharp bands present in both the sample and background spectra fail to ratio out properly. Typically, this is observed in the form of significant residual water-vapor absorptions in the spectrum. The way to correct for this is to make sure that the effective J-stop aperture is identical for both sample and background scans. This can be achieved at the expense of minimal loss of signal-to-noise ratio by selecting a J-stop with a diameter slightly smaller than the sample cell.

NOTE: *You can also use the $2cm^{-1}$ and $1cm^{-1}$ J-stops as reference aperture stops, as appropriate, for sample sizes less than 10 mm.*

Inserting a J-stop (Jacquinot Stop)

1 Hold the J-stop by its bent end, with the notched edge down (Figure 2-27).

2 Slide the J-stop into the grooves provided in the sample slide. As you push it toward the rear of the sample compartment, angle its far end slightly toward the left.

3 Push until the J-stop goes no farther.

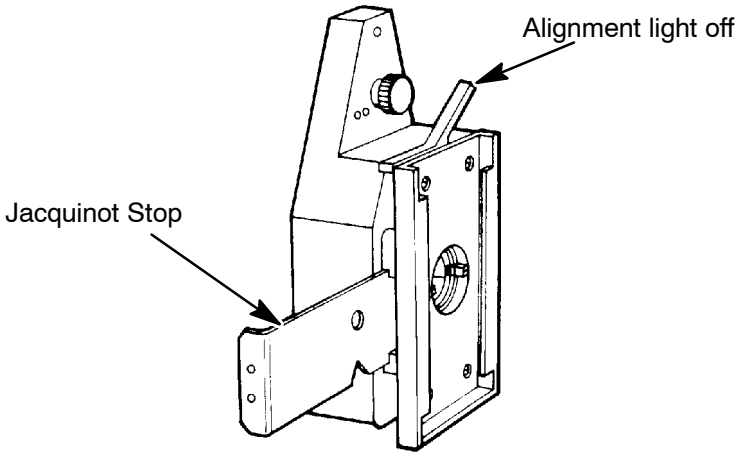


Figure 2-27 Inserting a J-Stop

4 Make sure that the aperture in the J-stop is centered in the opening of the sample slide.

Using the Alignment Light

You can use the sample slide as an alignment device for accessories, using the lever shown in Figure 2-27 to switch the alignment light on and off. Make sure that you switch it off completely before scanning. To align an accessory:

1 Install the accessory in the sample compartment.

2 Pull the lever on the sample slide towards you.
The alignment light is lit.

3 Adjust the accessory until the light is centered on the aperture in the right-hand side of the sample compartment.

4 Push the lever back to switch off the light.

Purging the Sample Compartment

There are two separate sets of connectors for purge gas lines, one for the sample compartment and one for the optical system. You can purge with either dry air or nitrogen. Either one removes water vapor; however, nitrogen is preferable because it also removes atmospheric carbon dioxide.

WARNING

Do not use a flammable gas to purge the Spectrum RXI. The Spectrum RXI contains a hot source, and a fire or explosion will result. Only use clean, dry, oil-free nitrogen or air to purge the instrument.

WARNING

Never connect the purge tubing directly to a gas cylinder or other high pressure supply; always use a pressure regulator and set the pressure to a maximum of 1 pound per square inch (6.9×10^3 Pa) before you start the flow.

Under most circumstances, you will never need to purge the optical system, and will rarely need to purge the sample compartment. You may want to purge the sample compartment if you need to make sure that no residual water vapor or CO_2 peaks are visible in the spectrum.

Purge gas enters the sample compartment through an inlet opening in the left side. No special outlet is necessary, the gas dissipates at the edges of the sample compartment cover.

1 Locate the tubing for sample compartment purge gas, which extends from the rear of the Spectrum RXI (Figure 2-28).

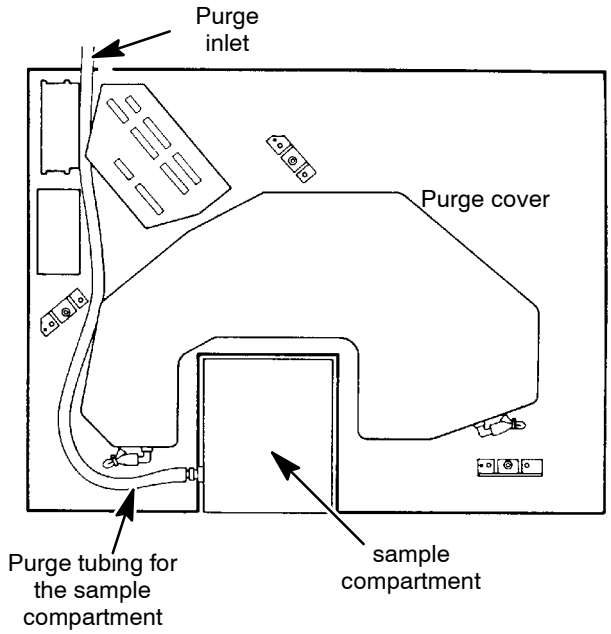


Figure 2-28 Purging the Sample Compartment

2 Connect this tubing to your source of dry nitrogen.

3 Set the flow rate for the gas at approximately 1 cubic foot per minute (28 L per minute).
The sample compartment is purged in approximately 2 minutes.

Using the Sample Shuttle

The optional sample shuttle moves the sample into and out of the infrared beam. Therefore, it is not necessary to open the sample compartment between collecting a background and the sample spectrum; this typically improves the cancellation of atmospheric features (CO_2 and water vapor) in the ratioed spectrum. The sample shuttle is suitable for lightweight samples such as card holders and sealed liquid cells; it is not intended to be used with bulky accessories. (*shuttle*) enables you to select one of three modes of operation for the shuttle:

- manual — To move the shuttle into or out of the beam, you press an action key (*in* or *out*).
- semi-automatic — The shuttle moves out of the beam automatically for background scans in ratio mode. For other scans, the shuttle moves into the beam, and remains there until you move it by pressing a soft key.
- automatic — In ratio mode, the Spectrum RXI automatically collects an equal number of background scans and sample scans. The shuttle moves out of the beam for the background scans. Otherwise, the shuttle remains in the beam, unless you move it by pressing a soft key.

NOTE: *(shuttle) is displayed at Ready For Next Command only when you have a sample shuttle plugged into the connector on the right-hand side of the sample compartment. If you unplug the shuttle, the key is no longer displayed.*

The factory default conditions for scanning with a sample shuttle are:

- scan mode - ratio
- shuttle mode - manual
- shuttle position - out of the beam when the Spectrum RXI is switched on.

The scan mode and shuttle mode are stored in battery-backed memory. When you switch it on, the Spectrum RXI is in the same scan and shuttle modes as when it was switched off. However, the shuttle is always out of the beam when you switch on the Spectrum RXI, irrespective of where it was when you switched off the Spectrum RXI. In semi-automatic mode, the shuttle moves out of the beam when you collect a background scan.

If you change the shuttle mode to automatic, the Spectrum RXI determines when to collect background scans:

- If you specify a relatively small number of sample scans, the Spectrum RXI collects that number of background scans, followed by the sample scans.
- For a larger number of sample scans, groups of background scans alternate with groups of sample scans.
- When you use the Monitor Scan command, sample and background scans automatically alternate.

Using the Shuttle Command

1 At Ready For Next Command, press **shuttle**.
The command line and soft keys in Figure 2-29 are displayed. The three soft keys on the left set the shuttle mode. **in** *and* **out** *move the shuttle.*

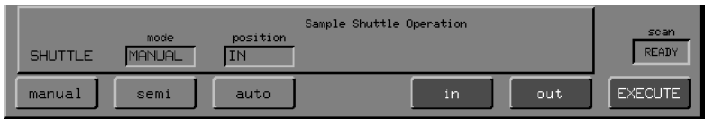


Figure 2-29 The Shuttle Command Line and Soft Keys

2 If you want to change the shuttle mode, press the appropriate soft key.
The **mode** *field changes to the new setting. If you do not want to move the shuttle, go to step 4.*

3 To change the position of the shuttle, press **in** *or* **out**.
The shuttle begins moving as you directed, and Ready For Next Command returns.

4 If you did not press an action key at step 3, press **EXECUTE**.
Ready For Next Command returns.

NOTE: *The detector must recover for a few seconds each time the shuttle changes position. If you enter a Scan command before this time elapses, the Spectrum RXI waits;* **START** *is displayed in the scan status box until the scan begins.*

Viewing and Processing 3

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Introduction

After you have collected a spectrum, you can view and process it. For example, you can expand and move the spectrum to view a small region of interest, use the cursors to determine the wavenumber position and ordinate value of a peak, and attach comments to the spectrum. Then you can, for example, flatten or smooth the baseline.

About This Chapter

Section	Starts on Page	Describes
Setting Up the View Options	3-2	how to set up the six View Options that control either the graphics display or the functions of specific View Keys.
Selecting a Spectral Region to View or Process through to *Viewing the Scroll Buffer*	3-14	how to use the View Keys
Some Notes About Processing	3-51	the range of execution, how to keep the original spectrum, and how to process a spectrum that has been stored on disk.
Abex through to *T/A*	3-53	why and how to use the Process Keys.

Setting Up the View Options

The View Options

You can set up six View Options (Table 3-1) that control either the graphics display or the functions of specific View Keys. (The other View Option — colors — is described in *User Preferences* in *Advanced Operations*.) The settings are not lost when you display text or a table, and they are stored in battery-backed memory, so they are retained even when the Spectrum RXI is switched off.

NOTE: *A spectrum or interferogram is displayed when you access one of the View Options. So, when you have changed a setting of one of the View options, you can manipulate the graphics and see the effect of the change before you* EXECUTE *the command.*

View Option	Function	Page
Autex	Selects either on-request vertical expansion, or automatic vertical expansion.	3-4
Hold	Selects the center of expansion that will be used when you vertically expand or contract the spectrum.	3-5
Peaks	Determines whether the peak cursor will move to maxima or minima, and sets a threshold peak value — to prevent the peak cursor finding noise.	3-6
Rerange	Sets the maximum and minimum values to which the abscissa range will be reset.	3-8
Rescale	Sets the maximum and minimum values to which the ordinate scale will be reset.	3-10
Schange	Switches on and off the 2:1 scale change on the display at 2000 cm^{-1}.	3-12

Table 3-1 The View Options in Setup

The factory default settings for the View Options are shown in Figure 3-1. To display them, press setup view .

Figure 3-1 Factory Default Settings of the View Options

Other View Parameters

Three other parameters affect the graphics display:

- the scan mode (single-beam, ratio, or interferogram), set in the Scan options of Setup (see page 2-26 of *Changing the Scan Options*);
- the ordinate mode (%T or A), set with T/A (see page 3-96);
- the abscissa range and ordinate scale, set with the horizontal and vertical arrow keys (see *Moving the Spectrum Horizontally*, starting on page 3-18, and *Moving the Spectrum Vertically*, starting on page 3-22).

Scan mode and ordinate mode

The scan mode and ordinate mode are stored in battery-backed memory. This means that if you have been viewing a ratio spectrum in %T and you switch off the Spectrum RXI, the next time that you switch it on, the displayed spectrum will be in ratio mode and %T.

Abscissa range and ordinate scale

These settings are not lost when you display text or a table, but they are lost when the Spectrum RXI is switched off.

Autex

The View Autex option determines the behavior of **autex**.

One-time autex

If View Autex is **OFF**, pressing **autex** expands the spectrum (*on-request*) so that it fills the entire screen vertically. The ordinate-scale limits change accordingly.

The new ordinate-scale limits are then used during all subsequent horizontal manipulations of the spectrum. They change only when you use the vertical display controls.

Continuous autex

If View Autex is **ON**, the spectrum is always expanded vertically to fill the entire screen. When you move the spectrum to the left or right with the horizontal arrow keys, the ordinate scale changes constantly as the spectrum expands or contracts to fit the screen. When this continuous autex is on, the ordinate scale limits are highlighted.

Continuous autex is temporarily switched off if you press any vertical arrow key; it is switched on again when you press **autex** or when you re-display a spectrum.

Setting the Autex option

1 At Ready For Next Command, press **setup** (**view**) (**autex**).
The command line and soft keys in Figure 3-2 appear.

Figure 3-2 The View Autex Command Line and Soft Keys

2 Choose a setting.

3 Press (EXECUTE) (EXIT).
Ready For Next Command returns.

Hold

[^ v] and [v ^] expand and contract the displayed spectrum vertically about a center. The View Hold option selects the center of this expansion and contraction as described in the following table:

Setting	Resulting Center of Expansion
bottom	level with the bottom tick mark on the ordinate axis
mid	level with the midpoint between the bottom and top tick marks on the ordinate axis
top	level with the top tick mark on the ordinate axis
auto	If no horizontal cursor is present, a baseline in the spectrum is used as the center of expansion. If a horizontal cursor is present, it becomes the center of ordinate expansion. If a vertical cursor is present, the intersection of the cursor with the spectrum is the center of expansion.

Table 3-2 Settings of View Hold

Setting the Hold option

1 At Ready For Next Command, press [setup] (view) (hold) .
The command line and soft keys in Figure 3-3 appear.

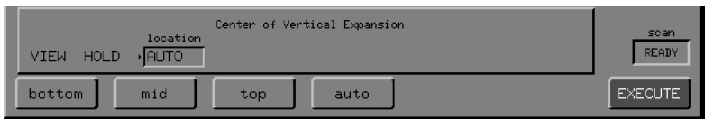


Figure 3-3 The View Hold Command Line and Soft Keys

2 Choose a setting.

3 Press (EXECUTE) (EXIT) .
Ready For Next Command returns.

Peaks

The View Peaks option controls the peak cursor. The option includes two parameters: the target and the threshold.

Target

Sets the peak cursor to find one of the following targets:

- **band** – band peak intensities (absorption maxima);
- **base** – baseline intensities to the side of absorbance bands (absorption minima);
- **both** – both at once.

Usually, transmittance peaks are assumed to be negative-going (point down) and absorbance peaks positive-going. However, if the **trans** Calculation option is switched on, the Spectrum RXI treats %T spectra like emission spectra, with positive-going peaks.

Threshold

This prevents the peak finder from finding noise.

When you change the threshold, the new value affects the behavior of the peak cursor only for the ordinate mode that is currently displayed. For example, if the spectrum on the screen is in %T, changing the threshold affects subsequent operation of the peak cursor with %T data. The Absorbance threshold does not change.

However, if you reset the threshold (and target) by pressing *reset*, the factory default values are restored at once for all data types. The factory default values for the threshold are as follows:

Ordinate Mode	Threshold
%T	2
Absorbance	0.01
Interferogram	2 Energy units
Single-beam	2 Energy units

Table 3-3 Factory Default Settings for Threshold

NOTE: *The View Peaks command also controls other functions involving peak-finding, in particular, the peaktable and height commands. When you are setting the target and threshold, make sure that you select the display mode that is appropriate to the peak-finding function that will be used: height always works in Absorbance, regardless of the display mode (unless the trans Calculation option is switched on), so make sure that the Absorbance threshold is set to an appropriate value.*

Setting the Peaks option

1 At Ready For Next Command, press **setup** (view) (peaks) .
The command line and soft keys in Figure 3-4 appear.

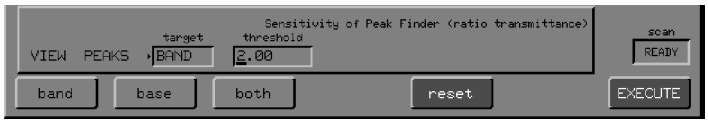


Figure 3-4 The View Peaks Command Line and Soft Keys

To restore the factory default target and threshold:

* Press (reset) (EXIT) .
Ready For Next Command returns.

To change the target or threshold:

a To change the target, press (band) , (base) or (both) .

b To change the threshold, type a number and press **enter** .

c Press (EXECUTE) (EXIT) .
Ready For Next Command returns.

Rerange

rerange resets the abscissa range limits of the display to their default values. The View Rerange option in Setup determines these defaults. That is, when you press **rerange**, you reset the abscissa range limits to the values set in the View Rerange option.

If you set new limits, they apply only to the data type currently on the screen (spectra or interferograms). However, you can restore the default abscissa range limits for *all* data types to their factory default values by pressing reset. These values are as follows:

Data Type	Rerange Limits
Spectra	4400 to 450 cm^{-1}
Interferograms	-500 to +500 μm (OPD)

Table 3-4 Factory Default Settings for Rerange Limits

Effect of changing the scan range

When you change the Scan Range option (see *Scan Options* on page 2-22), the same change is automatically made in View Rerange. This means that when you set the screen display at its default values, it subsequently displays the full range of your spectral data.

Setting the Rerange option

1 At Ready For Next Command, press **setup** (view) (rerange).
The command line and soft keys in Figure 3-5 appear.

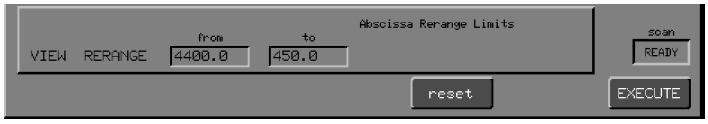


Figure 3-5 The View Rerange Command Line and Soft Keys

To restore the factory default:

* Press reset EXIT.
Ready For Next Command returns.

To enter new limits for the current data type:

a Type a number in the **from** field and press enter.
The cursor moves to the **to** *field.*

b Type a number in the **to** field and press enter.
The cursor returns to the **from** *field.*

c Press EXECUTE EXIT.
Ready For Next Command returns.

Rescale

rescale resets the ordinate scale limits of the display to their default values. The View Rescale option in Setup determines these defaults. That is, when you press rescale, you reset the ordinate scale limits to the values set in the View Rescale option.

If you set new limits, they apply only to the ordinate mode currently on the screen. However, you can restore the default abscissa range limits for *all* data types to their factory default values by pressing reset. These values are as follows:

Ordinate Mode	Rescale Limits
%T	0 to 100 %T
Absorbance	0 to 1.5 A
Interferogram	-100 to +100 (Power)

Table 3-5 Factory Default Settings for Rescale Limits

Setting the Rescale option

1 At Ready For Next Command, press setup view rescale.
The command line and soft keys in Figure 3-6 appear.

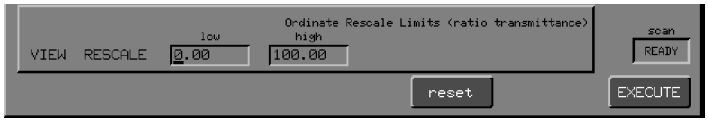


Figure 3-6 The View Rescale Command Line and Soft Keys

To restore the factory default:

* Press reset EXIT.
Ready For Next Command returns.

To enter new limits for the current data type:

a Type a number in the **low** field and press enter.
The cursor moves to the **high** *field.*

b Type a number in the **high** field and press enter.
The cursor returns to the **low** *field.*

c Press EXECUTE EXIT.
Ready For Next Command returns.

Schange

Representations of infrared spectra traditionally use a 2:1 scale change at 2000 cm^{-1}. This makes it easier to observe sharp bands in the fingerprint region, and compresses broad features above 2000 cm^{-1}. Figure 3-7 shows the same spectrum displayed with and without the scale change.

You can switch the scale change at 2000 cm^{-1} on and off.

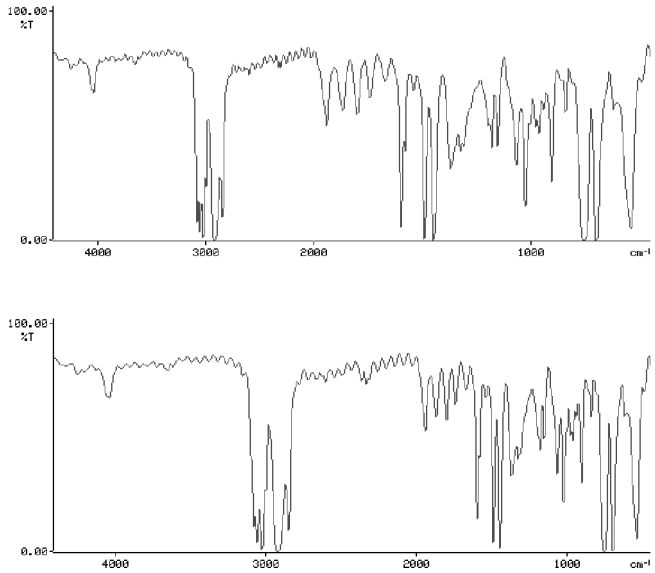


Figure 3-7 Spectrum Displayed with View Schange on (top) and off (bottom)

Setting the Schange option

1 At Ready For Next Command, press setup view OTHERS schange .
The command line and soft keys in Figure 3-8 appear.

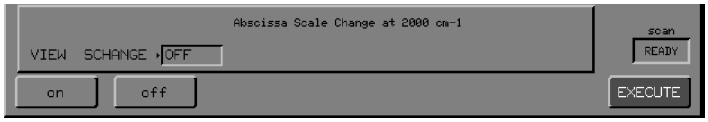


Figure 3-8 The View Schange Command Line and Soft Keys

2 Switch the scale change on or off .

3 Press EXECUTE EXIT .
Ready For Next Command returns.

Selecting a Spectrum Region to View or Process

The spectrum region keys correspond to the four memory regions — X, Y, Z and Backg(round) — in which the Spectrum RXI stores spectral data. By pressing a region key, you can:

- display the contents of that region. Pressing two or three region keys simultaneously displays the overlaid spectra of those regions — the rules for *Viewing More Than One Spectrum* are described on page 3-16.
- make that region the default region. This is the region that is used until you press another region key to change the default. If you press two or three region keys simultaneously, the first key of the press is the default region.
- switch on the graphical display if text has been displayed. (However, if a table is displayed, you cannot switch on either graphics or text.)
- enter that region into a field during a user interaction whose command line contains a **region** field.

Viewing One Spectrum

When you are viewing one spectrum, it is displayed as follows:

- The view range, scale and ordinate mode (transmittance or absorbance) are the same as those used the last time that you viewed a spectrum of that type.
- The axes are labelled with their ordinate and abscissa units. Table 3-6 shows the units for the various data types.
- The status line (below the spectrum) reports the region that you are viewing, the scan conditions, and any processing (such as **smooth**) that the spectrum has undergone (Figure 3-9). Also, a comment is displayed in this line if one has been attached to the spectrum.

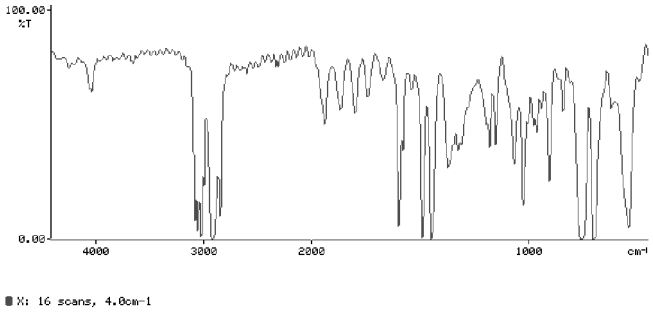


Figure 3-9 Viewing One Spectrum

Data Type	Abscissa Units	Ordinate Units
single-beam spectra	cm^{-1}	Spectral Energy (arbitrary units)
ratio spectra	cm^{-1}	%T
absorbance spectra (single or ratio)*	cm^{-1}	Absorbance units
raw interferograms	points	Volts
processed interferograms	OPD(μm)	Energy (arbitrary units)

Table 3-6 Labelling on the Axes

* The result of operating on a single-beam energy spectrum using T/A is not strictly an absorbance spectrum, but the logarithmic operation:

$-\log_{10}(E/100)$,

where E is in energy units.

This operation is closely analogous to the conversion of %T to absorbance. Nevertheless, with care, it is reasonable to infer absorbance differences (for example, peak to baseline) directly from the converted single-beam spectrum. Hence, for practical purposes, the ordinate is labelled in absorbance units.

Viewing More Than One Spectrum

Up to three compatible spectra can be displayed at one time, overlaid on the same set of axes. To display more than one spectrum, press two or three region keys simultaneously.

Figure 3-10 shows two compatible spectra overlaid. The display is similar to the display of a single spectrum, with the following exceptions:

- The first key that you press defines the default region.
- If continuous autoexpansion is switched on, the entire display is expanded to fill the screen.

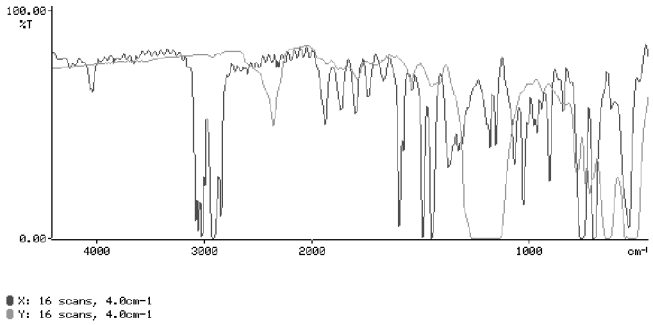


Figure 3-10 Two Compatible Spectra Overlaid On the Same Axes

Merging Spectra with Different Ranges

The total length of the scan range is limited to 4000 cm^{-1} at 1 cm^{-1} resolution, and to the entire range of the Spectrum RXI (7800 to 100 cm^{-1}) at resolutions from 2 cm^{-1} to 64 cm^{-1}. If you want a longer spectrum, collect two or three spectra of your sample over different ranges and display them together. For example, you could collect one spectrum from 7800 to 3780 cm^{-1} and another from 3800 to 100 cm^{-1}; when you display them together, the range is 7800 to 100 cm^{-1}. Overlap the scan ranges by 20 cm^{-1} so that there is not a gap between the parts of the spectrum.

Viewing Spectra of Different Types

Only spectra of the same type can be displayed together on the same axes. If you try to display incompatible spectra, note that:

- Interferograms can never be viewed with spectra.
- Single-beam and ratio spectra can be overlaid while you hold down both keys.
- While incompatible spectra are overlaid, each is displayed according to the current scale for that type.
- While incompatible spectra are overlaid, the axes are labelled according to the spectrum in the default region.
- When the simultaneous keypress ends, the default spectrum remains on the screen, with any other spectrum of the same type.

Background and ratio spectra

The most common reason to view incompatible spectra is to see the background spectrum (which is single-beam) overlaid on a ratio spectrum collected using that background. While you hold down **Backg** and the region key for the ratio spectrum simultaneously, both spectra are displayed.

Moving the Spectrum Horizontally

There are four arrow keys that you can use to move a spectrum horizontally:

◄	Moves the spectrum toward the left on the screen, or moves a vertical cursor to the left.
►	Moves the spectrum toward the right on the screen, or moves a vertical cursor to the right.
< >	Expands the spectrum horizontally about the center of the screen, or about a vertical cursor (see also page 3-26).
> <	Contracts the spectrum horizontally about the center of the screen, or about a vertical cursor (see also page 3-26).

Moving the Spectrum to the Left or Right

If you press ◄ or ► once, the spectrum moves toward the left or right of the screen, then stops. If you hold down the key, the spectrum continues to move, and accelerates, until you release the key. Moving the spectrum horizontally is often referred to as *panning*.

Effect on the axes

While the spectrum is moving horizontally, the usual abscissa axis labelling is replaced by endpoint values; it is redisplayed when you release the arrow key.

If automatic expansion is switched off, the ordinate scale does not change while the spectrum moves to the left or right. If continuous automatic expansion is on, the spectrum constantly expands and contracts vertically to fill the screen while the spectrum moves. The labels on the ordinate axis change accordingly. (To set up automatic expansion, see page 3-4.)

Limits of panning

The limits on panning to left and right are given in Table 3-7. Notice that these limits are wide enough to enable you to move a spectrum completely out of the display area.

Data Type	Upper Limit	Lower Limit
Spectrum (scale change on)	30766 cm^{-1}	-16384 cm^{-1}
Spectrum (scale change off)	16383 cm^{-1}	-16384 cm^{-1}
Processed interferogram	16384 μm	-16383 μm
Raw interferogram	16383 points	-16383 points

Table 3-7 Panning Limits

Horizontally Expanding and Contracting the Spectrum

Pressing [< >] or [> <] expands or contracts the spectrum horizontally about the center of the screen, or about a vertical cursor. The effect is to change the total range being displayed, called the *view range*.

Figure 3-11 shows a spectrum before using the expand and contract keys. Figure 3-12 shows the same spectrum expanded; note the shortened view range. Finally, Figure 3-13 shows the spectrum contracted; the view range is longer, actually beyond the limits of the data. (Scale change is **on** in all three displays.)

NOTE: *Horizontal expansion and contraction only affect the display, not data in memory. The original spectral data are all still available in the spectrum region. Moreover, if you shorten the view range before scanning, the scan still collects data over the entire range specified by the Scan Range option in Setup. You can then use the View Keys to see all the data collected.*

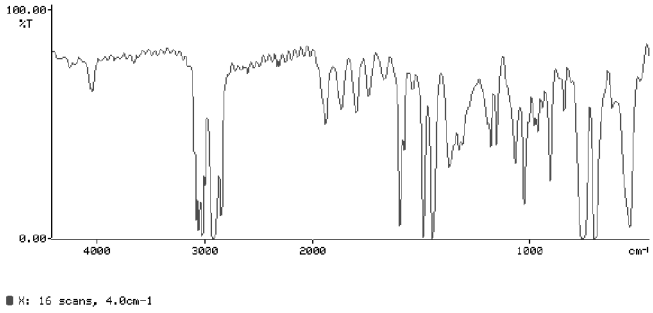


Figure 3-11 Original Spectrum

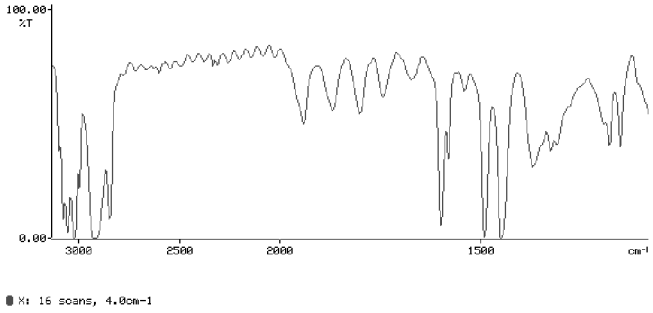


Figure 3-12 Spectrum After Abscissa Expansion

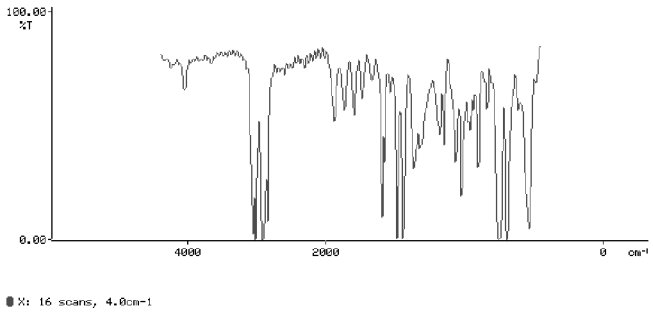


Figure 3-13 Spectrum after Abscissa Contraction

Reverse Entry

Before using the following commands, make sure that no graphics cursor is displayed.

Format	Example	Action
n ◄	**3500** ◄	Sets the upper limit of the view range to n cm^{-1}
n ►	**1000** ►	Sets the lower limit of the view range to n cm^{-1}
n < >	**5** < >	Expands the abscissa range by a factor of n
n > <	**5** > <	Contracts the abscissa range by a factor of n

Moving the Spectrum Vertically

There are four arrow keys that you can use to move a spectrum vertically:

Key	Function
↑	Moves the spectrum upward on the screen, or moves the horizontal cursor upward.
↓	Moves the spectrum downward on the screen, or moves the horizontal cursor downward.
⇕	Expands the spectrum vertically.
⇕	Contracts the spectrum vertically.

Moving the Spectrum Up and Down

Pressing ↑ or ↓ moves the spectrum up or down. As the spectrum moves, the ordinate scale is continually updated. If you hold down the key, the spectrum continues to move, and accelerates, until you release the key.

You can move the display vertically to:

- ±51 200 when a spectrum is in %T;
- ±256 when a spectrum is in Absorbance;
- ±51 200 when an interferogram is displayed.

Vertically Expanding and Contracting the Spectrum

Pressing ⇕ or ⇕ expands or contracts the spectrum vertically, and the center of this expansion or contraction is determined by the View Hold Option in Setup; the choices for the center are:

- the **top** tick mark on the ordinate axis;
- the **mid**point of the distance between the tick marks on the ordinate axis;
- the **bottom** tick mark on the ordinate axis;

- an **auto** setting, which enables the Spectrum RXI to determine a baseline to use as the center or, if a horizontal cursor is present, uses the position of the cursor.
- the intersection of a vertical cursor with the spectrum.

While the spectrum is expanding or contracting, scale labels on the ordinate axis update continuously. Figures 3-14, 3-15 and 3-16 show a spectrum that is first expanded vertically, then contracted.

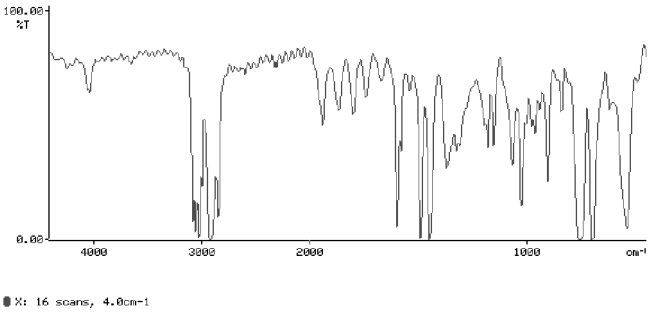


Figure 3-14 Original Spectrum

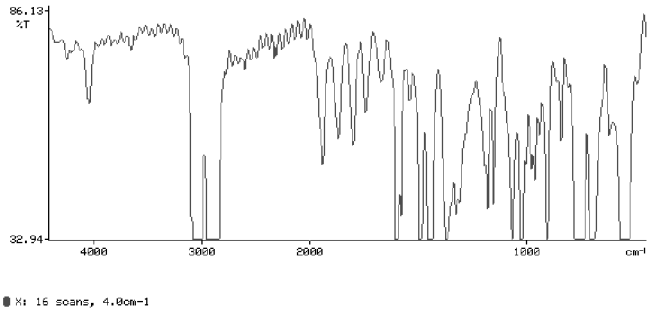


Figure 3-15 Spectrum after Ordinate Expansion

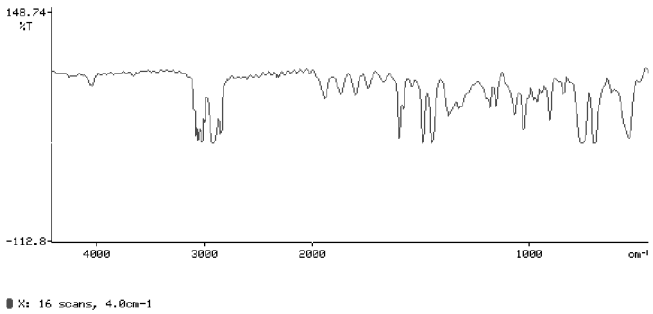


Figure 3-16 Spectrum after Ordinate Contraction

Reverse Entry

Before using the following commands, make sure that no graphics cursor is displayed.

Format	Example	Action
n ↑	**110** ↑	Sets the ordinate scale maximum to n, using the units currently displayed.
n ↓	**90** ↓	Sets the ordinate scale minimum to n, using the units currently displayed.
n ^ v	**5** ^ v	Expands the ordinate scale by a factor of n.
n v ^	**5** v ^	Contracts the ordinate scale by a factor of n.

Using the Vertical Cursor

You can use the vertical cursor to determine the wavenumber position and ordinate value of a peak. When the vertical cursor is displayed, the abscissa position of the cursor is reported under the label **vcursor**; the ordinate value at that position is reported in line with the spectrum status line of each spectrum that is displayed.

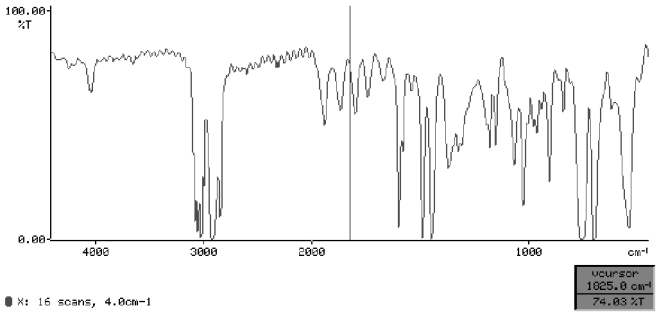


Figure 3-17 The Vertical Cursor Display

The vertical cursor has three main uses:

- If you press ***readcur*** when this cursor is displayed, the abscissa position of the cursor is entered in the command line (see page 3-34).
- ^ v, ^ v, < >, and > < use the cursor as the center of expansion and contraction where it intersects the spectrum.
- You can use it with < > to locate a peak and read its ordinate value.

Notes

◄ and ► move the vertical cursor to the left and right on the screen.

Two graphics cursors cannot be on the screen at the same time. If you press ***hcursor*** when the vertical cursor is displayed, the vertical cursor is removed and the horizontal cursor appears.

Using the Vertical Cursor

1 With a spectrum displayed, press **vcursor**.
A vertical cursor is displayed. The cursor data box is at the bottom right of the screen. The abscissa position of the cursor is reported under the label **vcursor***; the ordinate value at that position is reported in line with the spectrum status line.*

2 Press ◄.
The spectrum does not move, but the cursor moves to the left. The ordinate and abscissa positions are updated.

When the cursor reaches the extreme left of the display, it stops.

3 Press and hold down ◄.
The spectrum moves to the right.

4 Use ► to move the cursor back toward the center.

Determining an ordinate value

5 In the following steps, you use the vertical cursor to locate a peak and determine its ordinate value:

a Use ◄ and ► to move the cursor to a peak of interest.

b Use < > to expand the spectrum horizontally around the cursor.
The first time that you press < >, *the cursor and the peak under it move to the center of the screen. With subsequent presses, the peak expands very rapidly to make the maximum easy to find.*

c To expand the spectrum to fill the entire screen vertically, press **autex**. (For information about **autex**, see *Expanding the Spectrum to Fill the Display Vertically*, starting on page 3-41).

d Move the cursor to the left and right until the reported ordinate value is at a maximum.

e Use > < to slowly contract the spectrum. Confirm that you are on the peak.

6 Press **vcursor**.
The vertical cursor is removed.

7 Press **rescale** **rerange**.
The display returns to its default ordinate and abscissa limits.

Reverse Entry

Format	Example	Action
n **vcursor**	**2225 vcursor**	Moves the vertical cursor to exactly n cm^{-1}

Using the Peak Cursor

The peak cursor is a vertical cursor that jumps from peak to peak when you move it using ◄ and ►. This cursor is useful because the maximum (or minimum) ordinate value at the nearest peak is reported, even if that value does not fall on a screen pixel — you do not have to expand the spectrum to find the true peak value.

When you press ***peakcur***, a vertical cursor appears through the peak closest to the center of the display, as shown in Figure 3-18. This vertical cursor is labelled **peakcur** in the cursor data box. The ordinate value reported in the cursor data box, in line with the spectrum status line, is the minimum %T nearest to the cursor position. Pressing ***peakcur*** again switches the cursor off.

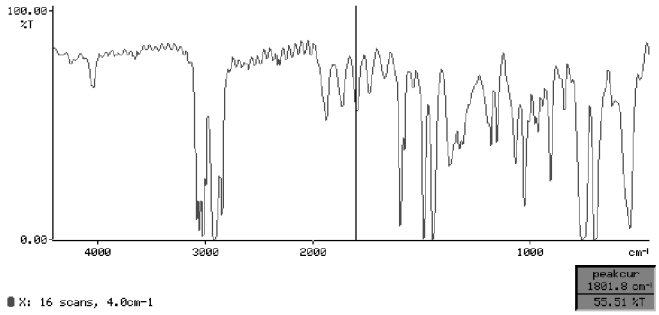


Figure 3-18 The Peak Cursor Display

Setup options The View Peaks options in Setup are:

- **target**. The peak cursor can search for **band** peak intensities, **base**line intensities at the sides of absorption bands, or **both**.
- **threshold.** The threshold prevents the peaks cursor from finding noise. The factory default thresholds are 2 %T, 0.01 A for spectra, and 2 energy units for interferograms.

Notes If you press ***readcur*** when the peak cursor is displayed, the abscissa position of the cursor is entered in the command line. At Ready For Next Command, you can list the abscissa positions of selected peaks in the command line: after you have pressed ***readcur***, press ***enter*** to enter a comma in the command line, then select another peak and repeat the procedure.

Two graphics cursors cannot be displayed at the same time. If you press ***hcursor*** or ***vcursor*** when the peak cursor is displayed, the peak cursor is removed and the new cursor appears.

When the peak cursor is displayed, < > and > < use the cursor as their center of expansion and contraction.

Using the Peak Cursor

1 With a spectrum or interferogram displayed, press ***peakcur***.
A vertical cursor appears at the peak nearest the center.

This vertical cursor is labelled **peakcur** *in the cursor data box. The ordinate value reported in the cursor data box is the minimum %T nearest to the cursor position.*

If more than one spectrum is displayed, the ordinate values are in line with the appropriate spectrum status line. The ▼ symbol in the cursor data box moves to identify the selected spectrum; the symbol is ▼ if transmittance spectra are displayed, and ▲ if absorbance spectra are displayed.

2 Press ◄.
The spectrum does not move, but the cursor moves one peak to the left. The values below the **peakcur** *label are updated.*

3 Press and hold down ◄.
The cursor moves to the left, jumping from peak to peak.

4 Use [→] to move the cursor back toward the center.

5 Press and hold down [< >].
The spectrum expands horizontally around the cursor.

6 Press and hold down [> <].
The spectrum contracts horizontally around the cursor.

7 Repeat steps 5 and 6, using [⇕] and [⇕].
The spectrum expands and contracts around the intersection of the peak cursor with the spectrum.

8 Press [peakcur].
The peak cursor is removed.

9 Press [rescale] [rerange].
The spectrum returns to its default ordinate and abscissa limits.

Reverse Entry

Format	Example	Action
n [peakcur]	**2225** [peakcur]	Moves the peak cursor to the peak closest to n cm^{-1}

Using the Horizontal Cursor

When the horizontal cursor is displayed, the ordinate position of the cursor is reported in the cursor data box, in line with the spectrum status line (Figure 3-19).

The horizontal cursor has two main uses:

- If you press **readcur** while this cursor is displayed, the ordinate position of the cursor is entered in the command line.
- If the View Hold Option in Setup is **auto**, vertical expansion and contraction using ^ v and v ^ are centered on the cursor.

NOTE: *To determine accurate ordinate values with the horizontal cursor, you must greatly expand the spectrum both horizontally and vertically. Preferably, use the vertical cursor or the peak cursor (see* Using the Vertical Cursor *on page 3-25 and* Using the Peak Cursor *on page 3-28).*

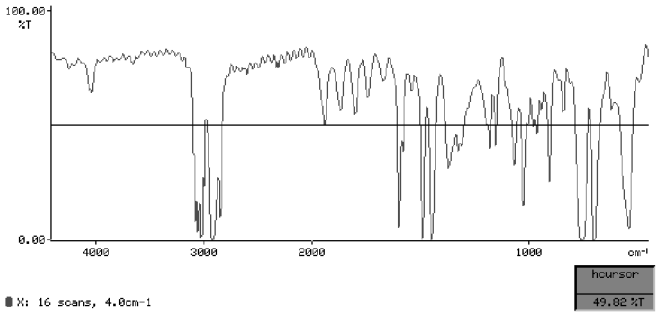


Figure 3-19 The Horizontal Cursor

Notes

Pressing **hcursor** toggles the cursor on and off.

↑ and ↓ move the horizontal cursor up and down.

Two graphics cursors cannot be displayed at the same time. If you press **vcursor** or **peakcur** while the horizontal cursor is displayed, the horizontal cursor is removed, and the new cursor appears.

Using the Horizontal Cursor

1 With a spectrum displayed, press **hcursor**.
The horizontal cursor appears in the center of the screen. The ordinate position of the cursor is reported in the cursor data box, in line with the spectrum status line.

NOTE: *If the vertical cursor was on the screen when you pressed* **hcursor**, *it is removed and the horizontal cursor appears at the intersection of the vertical cursor with the spectrum. If you then redisplay the vertical cursor, it is at the same abscissa position as before. This feature can be used, with the read cursor, to note both abscissa and ordinate values.*

2 Press ↑.
The spectrum does not move, but the cursor moves upward. The ordinate position in the cursor data box is updated.

Now you are going to prepare to use the horizontal cursor to enter an ordinate position, and as a center of vertical expansion.

3 At Ready For Next Command, press **setup** (**view**) (**hold**) (**auto**).
(Do *not* press EXECUTE yet.)
The horizontal cursor is now the center for vertical expansion.

4 Move the cursor to a suitable baseline position on the spectrum.

5 Press and hold down ⇕.
The spectrum expands around the cursor.

6 Press and hold down ⇕.
The spectrum contracts around the cursor.

7 If you do not want to use the view hold option **auto**, choose the setting that you want to use.

or

Press EXECUTE.
The View Options returns.

While you are in Setup, you can try using the cursor to enter an ordinate value.

8 Press **rescale** .
The command line shown in Figure 3-20 appears.

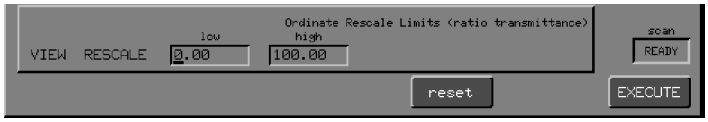


Figure 3-20 The View Rescale Command Line

9 Move the cursor down to a suitable lower limit for the scale, then press **readcur** .
The ordinate position of the cursor appears in the **low** *field.*

10 Press **enter** .
The alphanumeric cursor moves to the **high** *field.*

11 Move the horizontal cursor up to a suitable upper limit for the scale, then press **readcur** .
The ordinate position of the cursor appears in the **high** *field.*

12 Press **enter** .
The spectrum is rescaled.

13 To keep the previous values of the rescale limits, press **reset** .
The View Options are redisplayed.

14 Press **EXIT** .
Ready For Next Command returns.

15 Press **hcursor** .
The horizontal cursor is removed.

Reverse Entry

Format	Example	Action
n **hcursor**	**50** **hcursor**	Moves the horizontal cursor to the ordinate value n

Entering the Cursor Position in the Command Line

The current position of the graphics cursor (the horizontal, vertical or peaks cursor) can be entered in the command line by pressing ***readcur***.

- If the peak cursor or the vertical cursor is displayed, the abscissa position is entered.
- If the horizontal cursor is displayed, the ordinate position is entered.

Using the Read Cursor

Entering an ordinate value

1 With a spectrum displayed, move a vertical cursor (either the vertical cursor or the peak cursor) to the required abscissa position.

2 Press ***hcursor***.
The horizontal cursor appears at the ordinate value of the vertical cursor position.

3 Press ***readcur***.
The ordinate value is entered in the command line.

Entering an abscissa position

4 Now you will use the vertical cursor to enter an abscissa position:

a At Ready For Next Command, press ***setup*** ***view*** ***rerange***.
The command line shown in Figure 3-21 appears.

Figure 3-21 The View Rerange Command Line

b Move the cursor to the left, to a suitable upper limit for the range, then press ***readcur***.
The abscissa position of the cursor appears in the **from** *field.*

c Press ***enter***.
The alphanumeric cursor moves to the **to** *field.*

d Move the vertical cursor to the right, to a suitable lower limit for the range, then press ***readcur***.
The new abscissa position of the cursor appears in the **to** *field.*

e Press ***enter***.
The alphanumeric cursor moves to the **from** *field and the spectrum is reranged.*

f To keep the previous values of the rerange limits, press *reset*.

g Press *EXECUTE* *EXIT*.
Ready For Next Command returns.

Marking a Spectrum for Labelling

You use **mark**, with the vertical cursor or the peak cursor, to place marks on a displayed spectrum. Only a small vertical bar is displayed on the screen, but when you plot the spectrum, the marked peaks are labelled on the plot as specified in the Plot Peaks option of Setup (see page 4-19). The marks are displayed on the screen and in print-outs of the graphics display (Figures 3-22 and 3-23). You can place marks only within the range that is displayed, and there must only be one spectrum displayed.

mark is available whenever the View Keys are active; that is, you can mark a spectrum even during a user interaction or a scan.

Keeping and removing marks

Marks are not permanent; you can remove them from the screen at any time by pressing a region key, and they are lost when you save the spectrum to disk and then retrieve it. Marks are not removed when you:

- expand and contract the spectrum or move it to the left or right and up or down – the marks move with the spectrum.
- use a Process command (for example, Flat or Smooth), as long as you do not press a region key during the user interaction.

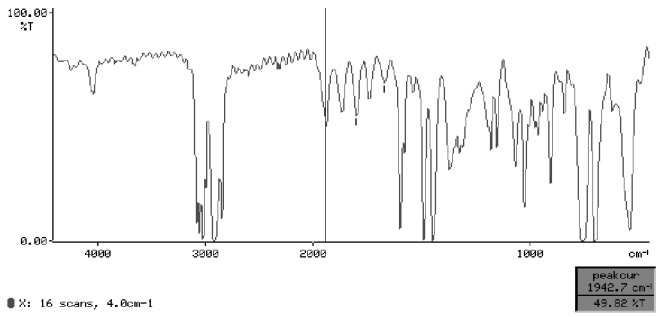


Figure 3-22 Marks on a %T Spectrum

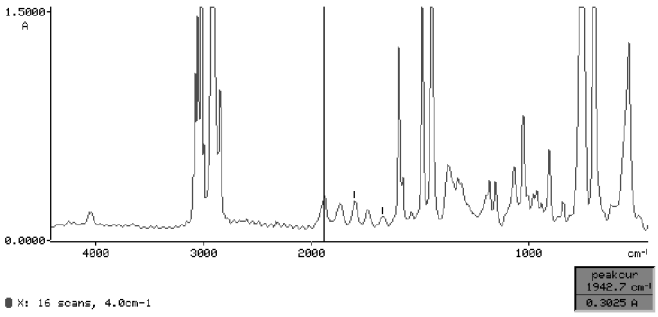


Figure 3-23 Marks on an Absorbance Spectrum

Marking a Spectrum

1 Display only the spectrum you want to mark.

2 Press ***vcursor*** or ***peakcur***.
The cursor appears.

3 Move the cursor to a position you want to mark.

4 Press ***mark***.

5 Move the cursor.
A vertical mark remains above or below the spectrum at the selected position.

6 Repeat steps 3 through 5 until all the required positions have been marked.

7 To clear the marks from the spectrum, press any region key, including the key of the displayed region.

Reverse Entry

Format	Example	Action
n ***mark***	**1350** ***mark***	Marks the spectrum at 1350 cm^{-1}.

Generating a Peak Table

A peak is an absorbance maximum or %T minimum that differs from the nearest valley by more than a threshold amount. The threshold is set by the View Peaks option of Setup.

Usually, transmittance peaks point down and absorbance peaks point up. However, if the **trans** Calculation option is switched on, %T spectra are treated like emission spectra, with peaks pointing up.

When you use **peaktable** as a Spectrum RXI command, it generates a list of the wavenumber positions and ordinate values of all the peaks in the specified range, as shown in Figure 3-24.

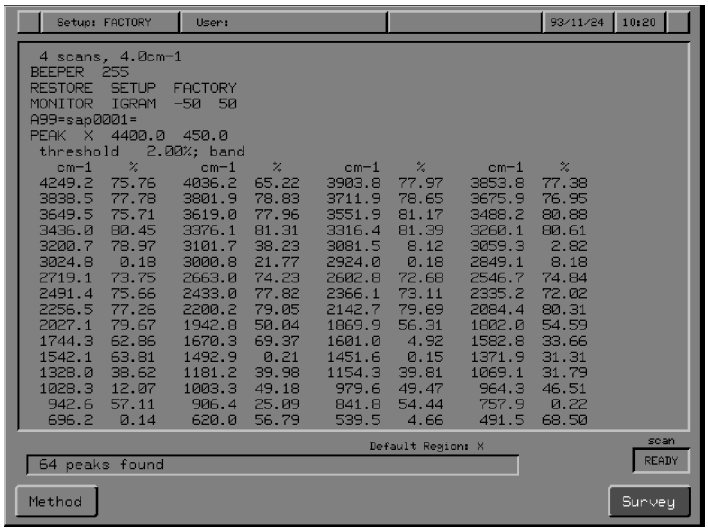


Figure 3-24 Typical Peaktable Generated by peaktable

Using peaktable

1 With the cursor at the beginning of the Command line, press ***peaktable***.
The command line and soft keys in Figure 3-25 appear. The entries for **region**, **start**, *and* **end** *are based on the current screen display.*

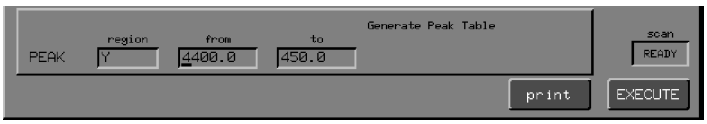


Figure 3-25 The Command Line and Soft Keys for peaktable

2 Press the keypad key for the region you require.
The **region** *field changes.*

3 Type the required upper limit in the **from** field and press ***enter***.
The cursor moves to the **to** *field.*

4 Type the required lower limit in the **to** field.

Executing peaktable

5 Press one of the two action keys that execute the command:

EXECUTE The peak table is displayed. If it contains fewer than 18 lines, it fits on the screen. To print the peak table, press ***print*** at Ready For Next Command.

print Outputs the peak table to both the screen and the printer. Use this method for tables longer than 17 lines.

A peak table is generated that is similar to Figure 3-24. The current settings of the View Peaks options are given at the beginning, and the total number of peaks at the end.

The position and ordinate value of the first peak are placed in ***V0*** *and* ***V1****, respectively. The total number of peaks is placed in* ***V2****.*

Using peaktable in expressions

Format	Examples
peak(x)=	peak(X)=
peak0(x)=	
peak1(x)=	
peak2(x)=	
peak0(x,w1)=	
peak1(x,w1)=	peak1(Y,2240)=
peak2(x,w1)=	
peak(x,w1,w2)=	
peak0(x,w1,w2)=	peak0(X,4400,2500)=
peak1(x,w1,w2)=	
peak2(x,w1,w2)=	

To find the ordinate value of the peak nearest to a given wavenumber, use the format: **peak1(x,w1)=**

Name of Result	Definition
peak or peak0	The abscissa position of the first peak found.
peak1	The ordinate value of the first peak found.
peak2	The total number of peaks found.

Expanding the Spectrum to Fill the Display Vertically

When you press **autex**, the displayed spectrum expands to fill the entire screen vertically. Only the display changes; the data in memory do not. (To multiply the data by an expansion factor, see *Abex* on page 3-53.) Figures 3-26 and 3-27 show the same spectrum before and after automatic expansion.

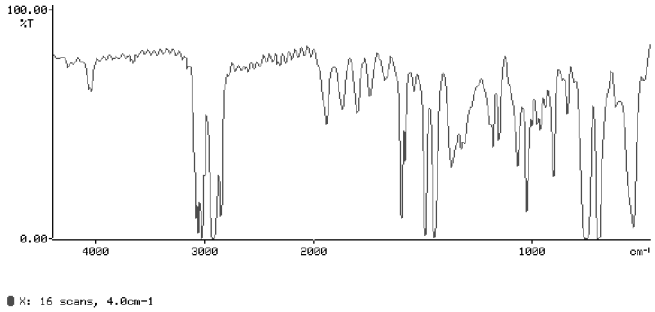


Figure 3-26 Spectrum before Automatic Expansion

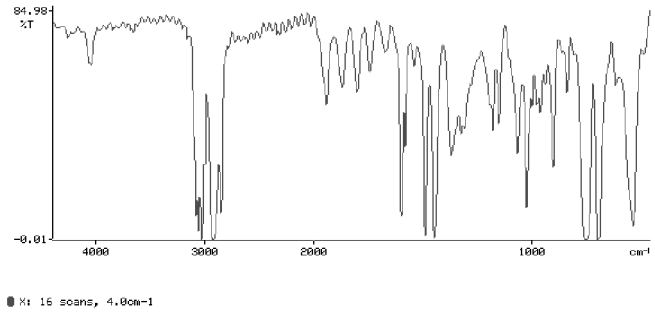


Figure 3-27 Spectrum after Automatic Expansion

autex works in one of two ways, depending on the setting of the View Autex Option:

One-time autex If View Autex is **OFF**, the spectrum is expanded on-request so that it fills the entire screen vertically.

Continuous autex If View Autex is **ON**, continuous automatic expansion is re-enabled (see steps 2 and 3 below).

Using Automatic Vertical Expansion

To see the behavior of both one-time autex and continuous autex, change the setting of the View Autex option in Setup:

1 With a spectrum displayed, press setup view autex.
The View Autex command line and soft keys appear. The spectrum is still displayed.

2 Press on.
Continuous automatic expansion is switched on, and the spectrum expands vertically. Note that the ordinate scale limits change, and that they are now highlighted.

3 Experiment with the displayed spectrum as follows:

a Use → and ← to move the spectrum horizontally.
The ordinate scale limits change as the spectrum moves.

b Press ↑.
The spectrum moves upwards.

c Now use → and ← again.
The ordinate scale no longer changes and the limits are not highlighted; the continuous autex has been temporarily disabled by pressing ↑ in step b.

d Press autex.
Automatic expansion is switched on again, as shown by the highlighted scale limits. Use → and ← to make sure that it is on.

The ordinate scale limits change.

NOTE: *Any change of vertical scale that conflicts with the automatic expansion temporarily disables continuous automatic expansion. Continuous automatic expansion is re-enabled when you press* **autex**, *or when a spectrum is redisplayed (for example, when you press a region key or the scan is updated).*

e Press **rescale** **rerange**.
The spectrum returns to its original appearance.

4 Press **off**.
Automatic expansion is switched off.

5 Experiment with the displayed spectrum as follows:

a Press **autex**.
The spectrum expands to fill the screen vertically. Note the new ordinate scale limits.

b Use ◄ and ► to move the spectrum horizontally.
The ordinate scale limits do not change.

c Press **rescale** **rerange**.
The spectrum returns to its original appearance.

6 Press either **on** or **off**, then press EXECUTE EXIT.
Ready for Next Command returns.

Resetting the Limits of the Displayed Spectrum

rerange and **rescale** reset the displayed spectrum to the default abscissa range and the default ordinate scale, respectively.

The default values are determined by the current settings of the View Rerange and View Rescale options in Setup. The factory-set default values are given in the following table, but you can set whatever default values are appropriate for your work.

	Units	Default Limits
Ordinate scale:		
	%T	0 to 100
	Absorbance	0 to 1.5
Abscissa range:		
	cm^{-1}	4400 to 450
	OPD (mm)	-500 to +500

Table 3-8 Factory-set Rerange and Rescale Values

Resetting the Limits

1 With a spectrum displayed, press horizontal arrow keys until you have changed the abscissa range considerably.

2 Press **rerange**.
The spectrum immediately returns to the default range.

3 Press vertical arrow keys to change the ordinate scale of the display.

4 Press **rescale**.
The spectrum returns to the default ordinate scale.

Attaching Comments to Spectra

You can attach comments to a spectrum that is in one of the spectrum regions. When you attach a comment to a spectrum, the comment becomes permanently associated with that spectrum. It stays with the spectrum when it is copied to disk or to a store region. The comment appears in the following places:

- on the graphics status line whenever the spectrum is displayed;
- in the caption when the spectrum is plotted;
- in the status information displayed when you use the Status command.

Notes

Comments can be up to 50 characters long.

You can also add comments to a spectrum when you copy the spectrum to disk.

If a comment is similar to the previous one, you can simply recall the previous one and edit it (see step 2).

Attaching Comments to Spectra

1 At Ready For Next Command, press ***comment***.
The command line and soft keys shown in Figure 3-28 appear. The soft key cursor is at the **region** *field, and there is no default entry.*

Figure 3-28 The Initial Command Line and Soft Keys for comment

2 Press a soft key to specify the data you want to identify, either a spectrum region or an lsf graph.
Your selection is entered in the **region** *field. If you chose a region, it is displayed, and the region soft keys disappear. (You cannot change the region. If you selected the wrong region, press* ***cancel*** *and begin again from step 1.)*

The alphanumeric cursor appears in the **comment** *field.*

3 Enter a comment.

* Type or edit a comment.

or

a If there is a (recall) soft key, you can create a new comment by editing the previous comment: press (recall).
The previous comment appears in the ***comment*** *field.*

b Edit the comment.

NOTE: *In a method file, combine steps 2 and 3 in the command* **COMMENT RECALL X***, where* **X** *represents the spectrum region you chose in step 2.*

4 Press enter
The comment is attached to the spectrum or lsf graph.

Ready For Next Command returns.

Displaying a Status Report

You can generate a description (the status report) of each spectrum region currently in the graphics display. The status report includes all of the following that exist:

- the conditions under which the spectrum was collected (scan range, maximum and minimum intensities, spectrum type, number of scans, resolution, mode, and apodization). Status reports for interferograms do not include resolution or apodization.
- the date and time the spectrum was collected.
- the spectrum name, if one has been assigned.
- a comment, if one has been added with **Copy** or **Comment**.
- the history of any manipulations that have been performed on the spectrum with the Process or Calculation Keys including date and time and the name of the operator, if a name was entered.

NOTE: *If a spectrum or interferogram is not displayed when you press* ***status****, the report describes the default region.*

Separate status reports are given for all spectra currently displayed.

To redisplay a spectrum or interferogram when a status report is displayed, press ***text****, any View Key, or any command whose interaction accesses graphics (for example,* ***scan*** *or* ***smooth****).*

To display a status report without the processing history, type **set history off** *and press* ***enter****, before pressing* ***status****.*

Displaying a Status Report

1 With a spectrum displayed, press **status**.
The spectrum is removed and a status report for the spectrum appears (Figure 3-29).

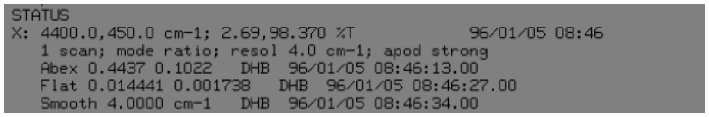


Figure 3-29 Typical Status Report for a Spectrum including History of Processing

2 Press **text**.
The spectrum reappears.

Viewing the Scroll Buffer

Commands that you previously executed, and the alphanumeric results of those commands, are stored in a region of memory in the Spectrum RXI called the scroll buffer.

Switching the Display between Graphics and Text

Pressing **text** toggles the display area of the screen between graphics and text.

- If graphics are on, the display area contains axes that display the contents of one or more of the four spectrum regions (Figure 3-30).

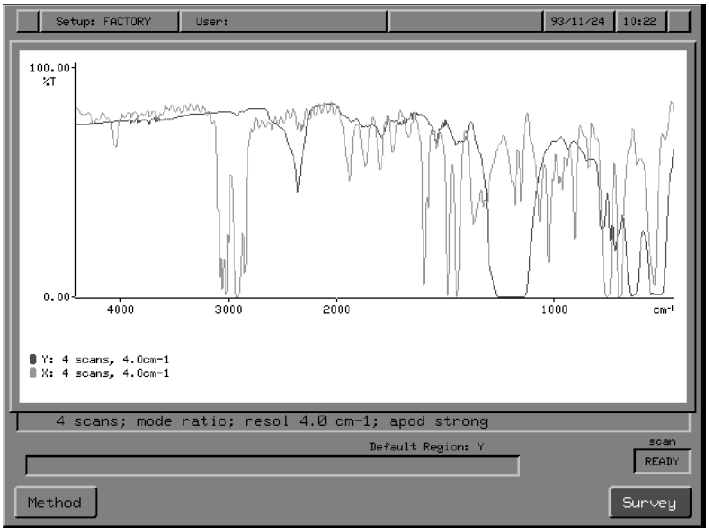


Figure 3-30 The Graphics Display of the Spectrum RXI

- If text is on, the display contains the scroll buffer, which lists commands, results, and error messages (Figure 3-31).
  The user interaction area of the screen remains at Ready For Next Command.

NOTE: *If a table of information is displayed,* **text** *does not work.*

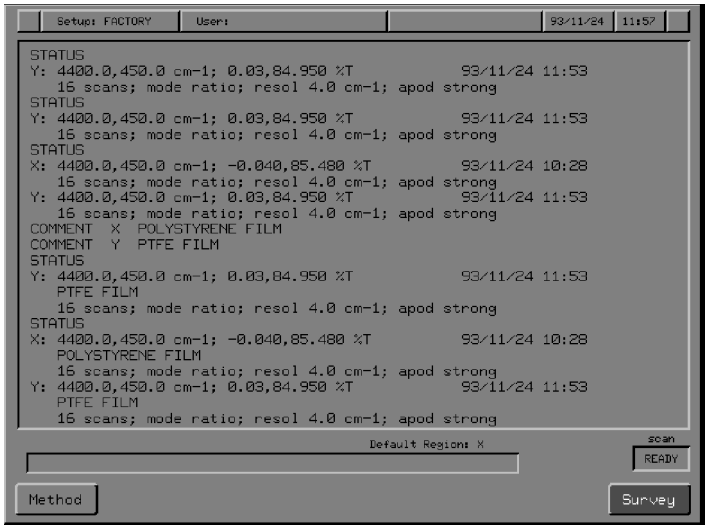


Figure 3-31 Spectrum RXI Text Display

Text

The command line and the Previous Command Line of the user interaction area are the last two lines of the line scroll buffer.

When the scroll buffer is full, the top line is lost each time a new line is added at the bottom. To save a printed copy of the buffer contents as they are generated, see page 4-29.

Some Notes About Processing

Range of Execution of Process Commands

Generally, when you execute a Process command, the entire spectrum is processed, even if only part of the spectrum is displayed.

NOTE: *You can specify the spectral range over which Flat is executed. If the Flat Range option of Setup is set to* **limited***, Flat executes only over a specified range; if Flat Range is* **full***, Flat executes over the entire spectrum.*

Keeping the Original Spectrum

When you use a Process command on a spectrum, the processed spectrum overwrites the original spectrum in the spectrum region. For example, if you Abex the spectrum in the X region, the result is placed in X. However, you can keep the original spectrum in any one of the following three ways:

- Copy the spectrum to another spectrum region or to a store region before you process it. This gives you a temporary copy of the original spectrum.
- Copy the spectrum to disk before you process it. This gives you a permanent copy of the original spectrum.
- If you forget to copy the data before processing, press ***restore*** to undo the Process command and restore the original spectrum to the spectrum region. Then copy the spectrum to another spectrum region, a store region, or disk before you process it again.

Processing a Spectrum That Has Been Stored on Disk

If the spectrum in a spectrum region was ever stored on disk, certain information has become permanently associated with it: a filename, a date, and possibly a comment and a user name.

When you process such a spectrum, the associated information is treated as follows:

Filename	Discarded, so you do not overwrite the original file when you save the processed spectrum.
Comment	Preserved. You can edit it when you save the processed spectrum.
User name	Replaced by the current user name. If there is not one, the original user name is preserved.
Date	Replaced by the current date.

Abex: Absorbance-expansion of a Spectrum

Using **abex** simulates the effect of changing the concentration or thickness of a sample, which is useful if you want to compare a spectrum with the spectrum of a reference material. In particular, when you compare two transmittance spectra, their band intensities must be similar otherwise the shapes of strong bands will appear different in the two spectra. If you are creating reference spectra, we recommend that you use absorbance expansion to normalize them and so make future comparisons easier: normalize the spectra by setting the intensity of the strongest band in every spectrum to a constant value, typically 1.5A, which is about 3%T. **abex** is most useful when the spectrum is weaker than you would like; if the sample is too thick, you cannot recover information from regions where the transmittance is essentially zero.

You can also use **abex** for simple baseline adjustment because it automatically sets the maximum transmittance to 100%. However, make sure that this maximum transmittance corresponds to a baseline point and not to a negative CO_2 contribution or to noise at the end of the spectrum. To adjust the baseline, set **factor** to **1**.

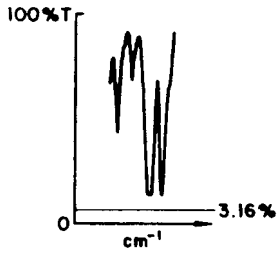
About Abex

You can expand the absorbance spectrum so that it fills the ordinate range, from 0 to 1.5 Absorbance units (or to a value other than 1.5 Absorbance units).

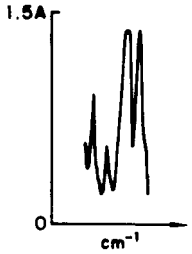
Although absorbance data are used for the Abex command, the graphics display will be in the current ordinate mode, either %T or absorbance.

How a spectrum is absorbance-expanded

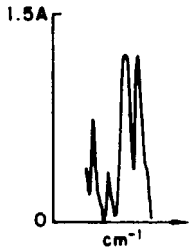
Absorbance expansion is a 5-step process:



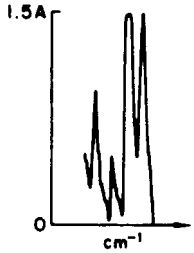
Spectrum A represents a %T spectrum. If the spectrum to be expanded is in %T, it is first converted to absorbance, giving spectrum B.



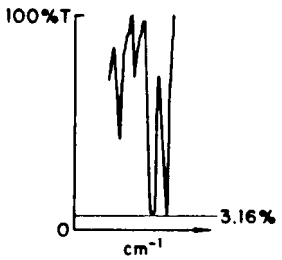
Spectrum B is in Absorbance. The difference between the minimum absorbance and zero is a baseline value that the system subtracts from the spectrum.



In **Spectrum C**, the subtraction has been performed, so that the minimum absorbance is now zero.



Spectrum D shows the effect of multiplying Spectrum C by an expansion factor. In this example, **auto** was pressed to expand the ordinate range to a maximum set by the expansion limit in the Abex Options of Setup (the factory default is 1.5 A).



In **Spectrum E**, the expanded spectrum is reconverted to %T. The maximum absorbance (1.5 A) has become the minimum transmittance, which is 3.16%T.

The expansion factor can be calculated automatically, or you can set it. Two setup options govern the behavior of an automatic Abex:

- The expansion limit is the **absorbance** range to which the spectrum is expanded. The factory default is 1.5 A.
- The **range** on which the Spectrum RXI bases the factor can be either the entire spectrum or only the displayed range. The factory default is the entire range. In either case, after the factor has been calculated, the entire spectrum is expanded.

Changing the behavior of Abex

1 At Ready For Next Command, press
setup *OTHERS* *OTHERS* *calc* *abex* .
The command line and soft keys in Figure 3-32 appear.

Figure 3-32 The Abex Option Command Line and Soft Keys

Changing the expansion limit

2 Type a number in the **absorbance** field.

Changing the search range

3 Press *full* or *limited* .

or

To use the current search range, press *EXECUTE* *EXIT* .
Ready For Next Command returns.

Expanding a Spectrum

1 Using the View Keys, display the spectrum region and the abscissa range you want to expand.
You can also adjust the screen display after step 2, or at any time during the following procedure until you execute the Abex command.

2 Press **abex**.
The Abex command line and soft keys appear (Figure 3-33).

The spectrum that is displayed corresponds to Spectrum C on the preceding page. The expansion factor is 1.

The **region** *is the spectrum region currently displayed. You can change it now by pressing a region key.*

Figure 3-33 Soft Keys and Command Line for Abex

3 Select the expansion factor in one of the following ways:

* Use the default factor (**1.0**).
* Type a new factor and press **enter**.
* Press **auto**.
* Use **more**, **less**, **faster** and **slower** to select a factor interactively.

4 Press **EXECUTE**.
The spectrum is absorbance-expanded, using the **factor** *in the command line, then:*

- *Ready For Next Command returns, with the expanded spectrum displayed.*
- *The graphics status line includes the word* **abex**.
- *The expansion factor is placed with the spectrum status information and in V-variable* **V0**.

Area: Area Under a Spectrum

The area function reports the area under a spectrum within a range that you specify. The area has the following units:

- %T.cm^{-1} for the transmittance area of a ratio spectrum;
- A.cm^{-1} for the absorbance area of a ratio spectrum;
- E.mm for areas of interferograms;
- E.cm^{-1} for areas of single-beam spectra.

Specifying absorbance or transmittance area

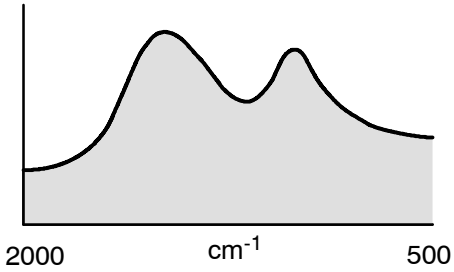
The area is calculated in absorbance or in transmittance, depending on the setting of **trans**:

- If the spectrum is displayed in absorbance, the area is calculated in absorbance
- If the spectrum is displayed in transmittance, the area is *still* calculated in absorbance, unless **trans** is switched to **on** (see page 3-98)

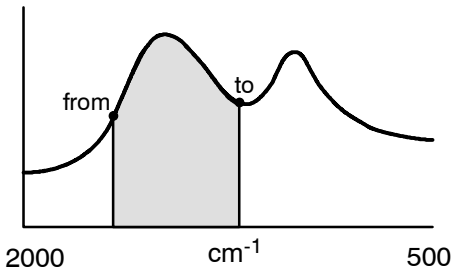
The title over the command line in the **area** user interaction tells you whether **area** calculates in absorbance or transmittance:

You usually need the absorbance area even if your spectrum is displayed in transmittance. However, the transmittance area is useful in applications that involve filters or anti-reflection coatings.

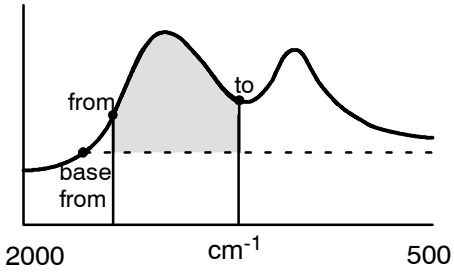
Specifying the area you require By changing the range over which **area** executes and by specifying different baselines (or none), you can vary the area calculated:



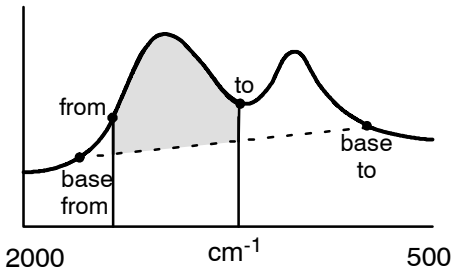
A: *area under entire displayed spectrum, down to the zero ordinate*- Use the default range (the range displayed on the screen) and do not specify a baseline.



B: *area under a specified range, down to the zero ordinate* - Specify a range but not a baseline.



C: *area down to a horizontal baseline* - Give both baseline fields the same value. (If **area** is calculating the absorbance area under a transmittance spectrum, the baseline appears curved.)



D: *area down to a slanted baseline* - Give the baseline fields different values.

Figure 3-34 Effect on the Area when the Range and Baseline Change

Restrictions on the range and baseline

The range and the baseline are each specified by two fields in the **area** command. The relationships among these four values are:

- The larger wavenumber (the leftmost abscissa) in each pair of fields must be given first. In the following example, the first pair of numbers specifies the range, the second specifies the baseline:
  area X 4000 3900 4200 3850
- All four numbers must be within the range of the spectrum.
- The numbers do not have to be within the limits of the screen display; for example, the baseline can extend off the screen.
- The baseline numbers can bracket the range numbers, be bracketed by them, or be to one side of them.

Using the area command

1 At Ready For Next Command, press **area**.
If the **trans** *Calculation Option of Setup is switched off, the command line and soft keys in Figure 3-35 appear. If* **trans** *is switched on, the command line and soft keys are as shown in Figure 3-36.*

The **from** *and* **to** *fields, which define the range over which* **area** *executes, contain the current limits of the displayed spectrum.*

If more than one spectrum is displayed, all except the spectrum in the default region are removed when you press **area**.

Figure 3-35 Command Line and Soft Keys for area if the trans Calculation Option is Switched Off

Figure 3-36 Command Line and Soft Keys For area
(with **trans** switched **on** and the ordinate displayed in %T)

2 To change the **region** field, press a region key.
The spectrum that is in the new region appears.

3 If you want to find the area under the entire displayed curve (A in Figure 3-34), go to step 11.

Specifying the range

4 To change the upper limit of the range, type a number in the **from** field. When the field is correct, press ***enter***.
The alphanumeric cursor moves to the **to** *field.*

5 To change the lower limit of the range, type a number in the **to** field. If you want the area for this range down to the zero ordinate (B in Figure 3-34), do not press ***enter*** but go to step 12.

6 Press ***enter***.

- If the **to** field is larger than **from** (for spectra), the cursor returns to **from**. Repeat steps 4 through 6 until **from** and **to** are correct.
- If **to** is smaller than **from**, the screen in Figure 3-37 appears.

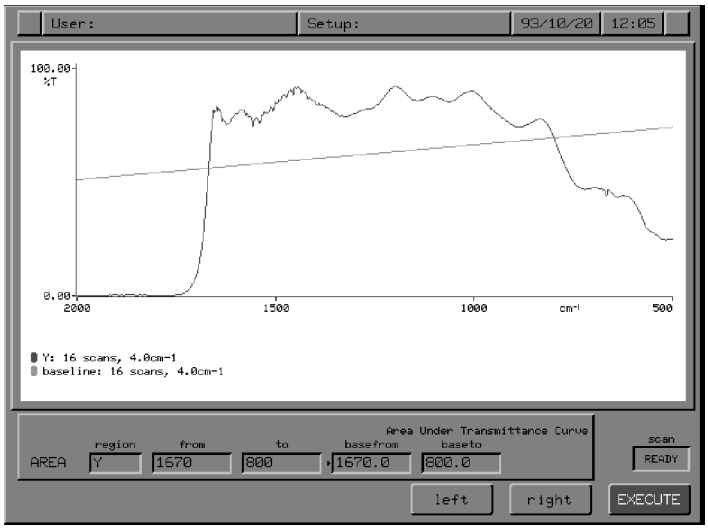


Figure 3-37 Default Baseline Drawn by the area User Interaction

- The **base from** and **base to** fields are filled in with the same values as **from** and **to**.
- The alphanumeric cursor moves to the **base from** field.
- A baseline is drawn on the spectrum from **base from** to **base to**.
- *left* and *right* appear.

Changing the two base fields

7 If the alphanumeric cursor is not in the **base** field that you want to change, press *enter*.
The cursor moves to the other field.

8 Type the wavenumber you want, or use a vertical cursor and *readcur* to enter the wavenumber. Press *enter*.
The baseline is redrawn to extend through the new position.

or

Move the end of the current baseline with *left* and *right*. If the cursor is in the **base from** field, the keys move the left-hand end of the baseline. If the cursor is in **base to**, they move the right-hand end.

While you hold down the soft key, the baseline extends only between the two "base" points (Figure 3-38). When you release the soft key, the baseline is extended across the screen.

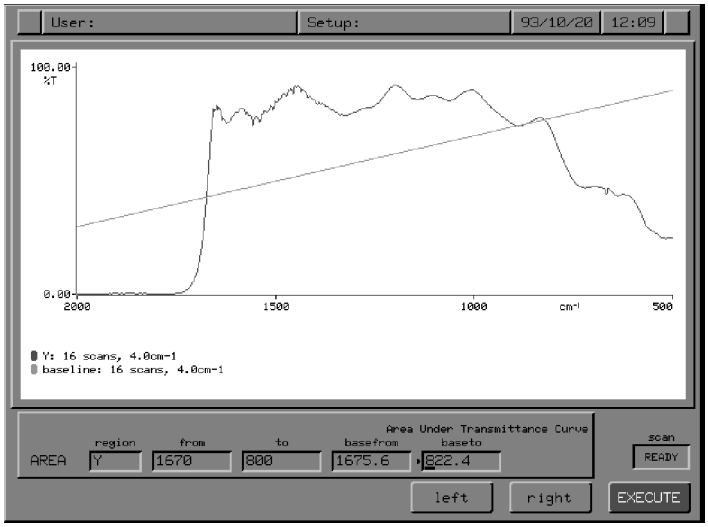


Figure 3-38 Drawing a Baseline with the area User Interaction

9 Repeat steps 7 and 8 until the baseline is where you want it.

Using a horizontal (flat) baseline

Refer to Figure 3-39 and C in Figure 3-34.

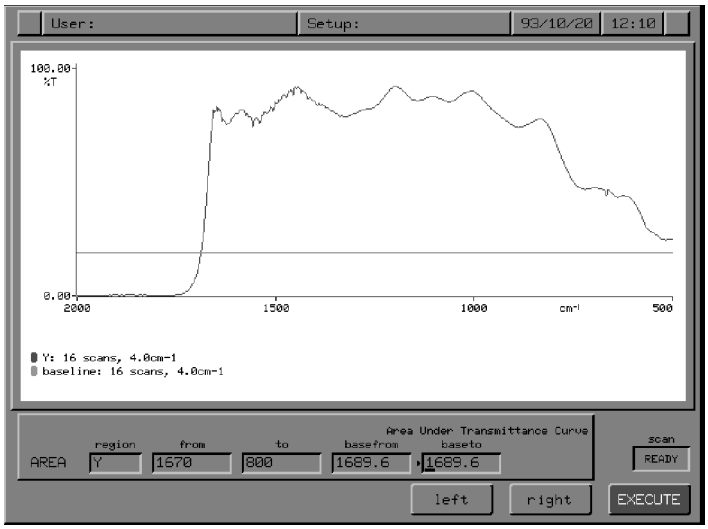


Figure 3-39 Horizontal Baseline Drawn with the area User Interaction

10 Make the two **base** fields the same. Do this in any of these ways:

* With the alphanumeric cursor in the **base from** field, press and hold down (right) until the left-hand end of the baseline reaches the right-hand end.

  or

* Type the same number in both **base** fields.

  or

a Use [readcur] to enter the same vertical cursor position in both fields.
A horizontal baseline appears at the position entered in the **base** *fields.*

b Move the baseline with (left) and (right).
The entire baseline moves, remaining horizontal as it does so.

11 If you want to change the **from** and **to** fields after you have entered the baseline points, press the region key of the spectrum that is displayed. For example, if you are working with a spectrum in the Y region, press [Y].
The alphanumeric cursor moves back to the **from** *field, but the* **base** *fields do not change. You can enter new values for* **from** *and* **to**.

Executing area

12 When the area that you want to calculate is specified, press (EXECUTE).
The area appears on the Command line and is assigned to variable **V0**. *The baseline is removed from the display.*

NOTE: *If the area you are determining is extremely small, it may not be possible to display all the significant figures in a labelled result. To see the entire result, type* **V0=**

The area saved in **V0** *is displayed according to the format set in the* **display** *command.*

Using area in an expression

In the formats listed below, b1 and b2 are points that define a baseline above which the area is to be calculated.

If you enter a value for b1 twice, without a corresponding b2, the baseline is a horizontal line through b1.

Format	Examples
area(x)=	area(Z)=
area(x,w1,w2)=	area(X,1800,1725)=
area(x,w1,w2,b1,b1)=	area(X,1800,1725,2000,2000)=
area(x,w1,w2,b1,b2)=	area(Y,1800,1725,2000,1600)=

Compare: Correlating and Comparing Two Spectra

The **compare** command compares a sample spectrum with the spectrum of a known compound (spectrum 1) and computes a correlation coefficient and a difference factor. It saves the correlation and the difference factor in the V-variables V0 and V1.

The calculations for compare are performed in absorbance whether the spectrum is displayed in %T or A. However, if your particular application requires transmittance calculations, you can change this (see *Processing Data in Transmittance*, on page 3-98).

NOTE: *The spectra must be collected at the same resolution.*

Comparing a spectrum with a spectrum on a disk

If the comparison is with spectra on disk, spectrum 1 is the spectrum on the disk that is most like the sample spectrum. Spectrum 2 is the spectrum next most like the sample.

When **compare** has finished, the spectrum on the disk that has the best correlation is placed in the restore region (see *Restoring a Spectrum to a Region* on page 2-20).

When you compare a sample spectrum with the spectra on a disk, a table similar to the one shown in Figure 3-40 is displayed. It shows the results for the fourteen spectra on the disk that are most like the sample spectrum. During the comparison, the bottom line reports the comparison currently in progress; it may or may not eventually be placed in the table, depending on how well it correlates with the sample.

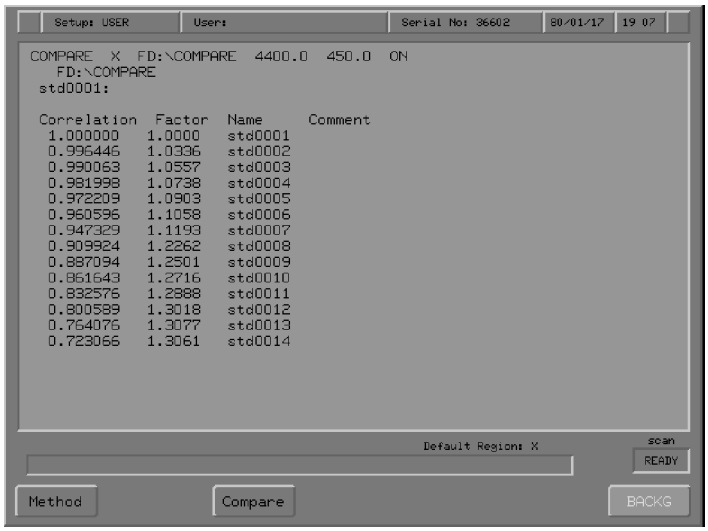


Figure 3-40 Table Generated when you Compare a Sample Spectrum with the Spectra on a Disk

The correlation coefficient

The Spectrum RXI calculates the correlation coefficient using the following equation:

$$r = \frac{X.Y}{(X.X)^{1/2} \times (Y.Y)^{1/2}}$$

The terms X.Y, X.X, and Y.Y are dot products.

Correlation coefficients range from zero to one:

- A correlation of zero indicates that the two spectra are completely unrelated. This, too, is unlikely in practice, because *all* absorption spectra have at least the similarity that absorption bands reduce the transmittance.
- A correlation of one is a perfect match. It is unlikely to occur unless the comparison spectrum is a copy of the sample spectrum.

The value for the correlation coefficient above which two spectra can be considered identical depends on the methods and care used to obtain them. Typical thin film absorbance spectra of replicate samples may correlate to better than 0.999. However, you should establish numerical criteria experimentally for each set of conditions.

The difference factor

The difference factor is calculated from the absorbance spectra. It gives the number by which you must multiply the comparison spectrum in order to give the closest fit to the sample spectrum (in absorbance).

To demonstrate the differences between the sample spectrum X and the comparison spectrum Y:

1 Use **compare** to determine the difference factor.

2 Use **Diff** with the factor determined in step 1. For example, if the factor was 1.2, the command would be: **diff X Y Z 1.2**
The result spectrum in region Z shows the features that are not common to X and Y.

Filtering

The filter option enables compare to give relatively more weight to aspects of the data likely to reflect genuine differences between the samples. It gives less weight to differences probably caused by experimental factors such as sample preparation methods or instrument conditions.

Filtering is on by default. If you switch it off, compare exaggerates differences that may not be significant. Nevertheless, if you do your own processing of the spectral data, you may want to switch the filter off.

Various types of filtering are available, as described in Table 3-9. To select one type, you enter its selection number in the compare command line. To select more than one type, you enter the *sum* of their selection numbers.

NOTE: *Options 8 through 32 are ignored if option 4 is not selected; also, option 1 is ignored if option 4 is selected.*

Selection	Description of Filter
0 or OFF	*No filter*
1 or ON	*Default filter:* equivalent to selecting 2, 4, and 8, below.
2	*Resolution weighting:* emphasizes spectral features that occur at a resolution of about 16 cm^{-1}. Features at higher resolutions than this tend to be noise, while low resolution features tend to be baseline curvature or slope.
4	*Black band/black body weighting:* black band weighting emphasizes absorbance peaks near 0 Absorbance more than peaks that are near infinite absorption. This is because compare uses absorbance spectra, and black bands can have a significant absorbance error. Black body weighting emphasizes the absorbance values in the high fingerprint region, which have higher signal-to-noise ratios than those at either extreme of the mid-infrared region.
8	*CO_2 suppression:* excludes bands from 2390 to 2280 cm^{-1} and the band at 667 cm^{-1}.
16	*Deweighting of water regions:* deweights the regions from 4000 to 3500 cm^{-1} and from 1900 to 1300 cm^{-1} by a factor of 8.
32	*Full blanking of water regions:* excludes completely the regions from 4000 to 3500 cm^{-1} and from 1900 to 1300 cm^{-1}.

Table 3-9 Filters Used by Compare

Setting up the compare location

If you are comparing the sample spectrum with the spectra on a disk, you can specify the default disk directory that is entered in the Compare command line when you press (disk).

1 Press setup (OTHERS) (OTHERS) (compare).
A directory tree and the soft keys for choosing the Compare location are displayed.

2 Enter the required directory name in the **region** field.

3 Press EXECUTE.
Ready For Next Command returns.

Using compare

1 At Ready For Next Command, press ***compare***.
The command line and soft keys in Figure 3-41 appear, with the cursor at the first **region** *field.*

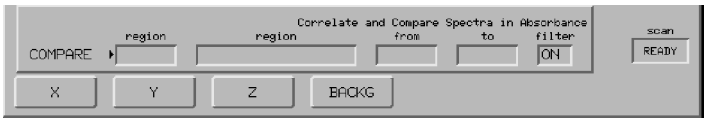


Figure 3-41 Command Line and Soft Keys for Compare

2 Press the soft key for the region that contains the sample spectrum.
The cursor moves to the second **region** *field. A* **disk** *soft key is displayed in addition to the region soft keys.*

3 Press the soft key that represents the location of the spectrum or spectra to be compared with the sample spectrum (Figure 3-42). If you want to use a spectrum that is stored on the floppy disk, press ***disk***, then press ***newpath*** to choose a different directory.
If you are comparing the sample spectrum with a single spectrum, **from** *and* **to** *are filled in with the range in which the two spectra overlap. If you are comparing the sample spectrum with the spectra on a disk,* **from** *and* **to** *contain the range of the sample spectrum.*

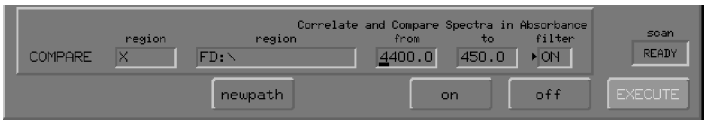


Figure 3-42 Command Line and Soft Keys after Both region Fields are Filled

4 If you want to change the upper limit of the range, type a new number in the **from** field. Press ***enter*** when the field is correct.
The cursor advances to the ***to*** *field.*

5 If you want to change the lower limit, type a new number in the **to** field.

6 Press on or off, or type the selection number of the filter that you want to use.
You can use several filters together by typing the sum of their selection numbers.

7 When the command line is correct, press EXECUTE.
The result of comparison with a single spectrum is displayed on the Command Line; results of comparisons with spectra on a disk are displayed in the display area.

Ready For Next Command returns.

Diff: Generating a Difference Spectrum

The Diff command subtracts one spectrum from another. By calculating the difference between two spectra, you can remove the contribution of some components and see what remains. For example, you might subtract the spectrum of the solvent from that of a solution.

You can optimize the elimination of particular bands by varying a scaling factor that is applied to one of the spectra. Diff works in absorbance because it is the absorbance that varies linearly with concentration or path length. If the spectra include regions where the absorbance is very high, the noise level in these regions of the difference spectrum will be high. Difference spectra are very sensitive to small changes in the shapes and positions of bands: you should use identical instrument conditions for the two spectra involved in any subtraction.

Description

Because you often obtain the mixture spectrum and the component spectrum at different concentrations or sample thicknesses, they must be brought into the same scale. This is done by multiplying the component spectrum by a factor:

mixture – (component * factor) = difference

You can determine the appropriate factor interactively, or the factor can be calculated automatically.

When you execute Diff, the value of the factor is placed with the status information for the spectrum and in V-variable V0.

Ordinate mode of the difference spectrum

The calculations for Diff are performed in absorbance whether the spectrum is displayed in %T or A. If your application requires transmittance calculations, see *Processing Data in Transmittance*, on page 3-98.

The difference spectrum is displayed in the ordinate mode (either absorbance or %T) of the spectra from which it was calculated. If the two source spectra are in different modes, the difference spectrum is in the same mode as the spectrum in the second **region** field.

When the source spectra are not compatible

Difference spectra are most meaningful when the two source spectra are of the same range, resolution, apodization, and type (ratio, single-beam, or interferogram). However, you can use Diff in the situations listed in the following table, after clearing a warning message.

Problem	Explanation
Type Mismatch	One source spectrum is single-beam, the other is ratioed.
Resolution Mismatch	The two spectra have different resolutions. However, either both have resolutions of 4 cm^{-1} or more, or both resolutions are less than 4 cm^{-1}.
Apodization Mismatch	The two source spectra were collected using different apodizations.

Table 3-10 Situations that Generate a Warning in Diff

The situations listed below involve source spectra that are so mismatched that the Spectrum RXI cannot manipulate them together. An error message appears, and you should either cancel the command or choose a different combination of spectra.

Problem	Explanation
Type Mismatch	One source is an interferogram, the other is a spectrum.
Range Mismatch	The two source spectra are of different wavenumber ranges.
Resolution Mismatch	One source spectrum has a resolution less than 4 cm^{-1}, the other is 4 cm^{-1} or more.

Table 3-11 Situations that Generate an Error in Diff

Using the Diff Command

1 Press **diff**.
The Diff command line and soft keys appear. The soft key cursor is at the **region** *field, but there is no default entry. The alphanumeric cursor is at the* **factor** *field, with a default entry of* **1.0**.

Figure 3-43 Initial Command Line and Soft Keys for Diff

2 Choose the region containing the spectrum of the mixture by pressing **X**, **Y**, **Z** or **BACKG**.
*The spectrum appears. The soft key cursor moves to the next field (***region * factor***).*

3 Choose the region containing the spectrum of the pure component by pressing **X**, **Y**, **Z** or **BACKG**.
The spectrum of the component is displayed, and the soft key cursor moves to the **destination** *field.*

4 Choose the region to receive the difference spectrum, by pressing **X**, **Y**, **Z** or **BACKG**.
The current contents of the region appear briefly, so that you can see the data that will be overwritten. Also, if the destination is BACKG, a message appears, **WARNING: Current background will be overwritten**.

The soft keys change to those shown in Figure 3-44. The calculated difference spectrum, based on a default factor of 1, appears.

Figure 3-44 Soft Keys for Determining the Factor in Diff

5 Use the horizontal view keys to adjust the range of the displayed spectrum, if you need to.

NOTE: *The following is a helpful approach to using Diff when there is an obvious peak to be eliminated:*

a Expand the spectrum until only that peak is displayed.

b Press (auto).
A factor that eliminates the peak is calculated.

c Contract the spectrum to the original range to see the result.

d Select the factor in one of the following ways. As you adjust the factor, use the View Keys to help you follow the peak that is of most interest.

* Use the default factor (**1.0**).
* Type a value, and press [enter].
* Press (auto).
The Spectrum RXI selects a factor based on a least squares fit of the pure component spectrum to the mixture spectrum.
* Use (more), (less), (faster) and (slower) to select a factor interactively.

e Press (EXECUTE).
The Diff calculation is performed, using the factor specified. When the computation is complete, the following actions occur:

- *The difference spectrum is displayed in the ordinate mode (%T or A) of the original spectra, or in absorbance if the two source spectra were in different ordinate modes.*
- *Ready For Next Command returns.*
- *The graphics status line includes the word* **diff**.
- *The two original source spectra are unchanged.*
- *The Diff factor is placed with the spectrum status information and in V-variable V0.*

Flat: Correcting the Baseline

Flat removes broad baseline features from spectra. It is most useful for very weak spectra, where large ordinate scale expansion may be needed to see the peaks.

Flat can be used to reduce the background due to scattering in spectra of solids prepared as mulls or disks. However, remember that when there is a lot of scattering you may get distorted band shapes. Flat is not a substitute for good sample preparation.

When Flat corrects a baseline, the calculation is done in absorbance and the peak intensities are unchanged. You can use Flat for baseline correction within a quantitative method.

About Flat

In Setup, you can set the following Flat Options:

- the number of orders of baseline correction. The factory default is two orders, **slope** and **bow**. However, you can add to or reduce the number of orders while you are in the Flat user interaction. Thus, you can decide to use one, two, three, or four orders of baseline correction, irrespective of the setting of the **# Terms** option in Setup.

NOTE: *You can add a field to Flat while you are using the command by pressing* shift (next) *when the cursor is in the right-hand field.*

- the range over which the baseline correction is to be performed, either the full range of the spectrum or a limited range. The factory default is **full**.

The calculations for Flat are performed in absorbance whether the spectrum is displayed in %T or A. If your application requires transmittance calculations, see *Processing Data in Transmittance* on page 3-98.

Orders of baseline correction

The Flat command line contains up to four numeric fields. These fields represent the possible orders of flattening you could apply, and are called **slope**, **bow**, **skew**, and **wave**. The numbers in each field are proportional to the ordinate distances represented by d in Figure 3-45. The greater the value of d, the greater the correction applied.

When Flat executes, the values for all the numeric fields on the screen are added to the status information for the spectrum. They are also placed in the V-variables; beginning with V0, as many of the variables V0...V3 as necessary are used.

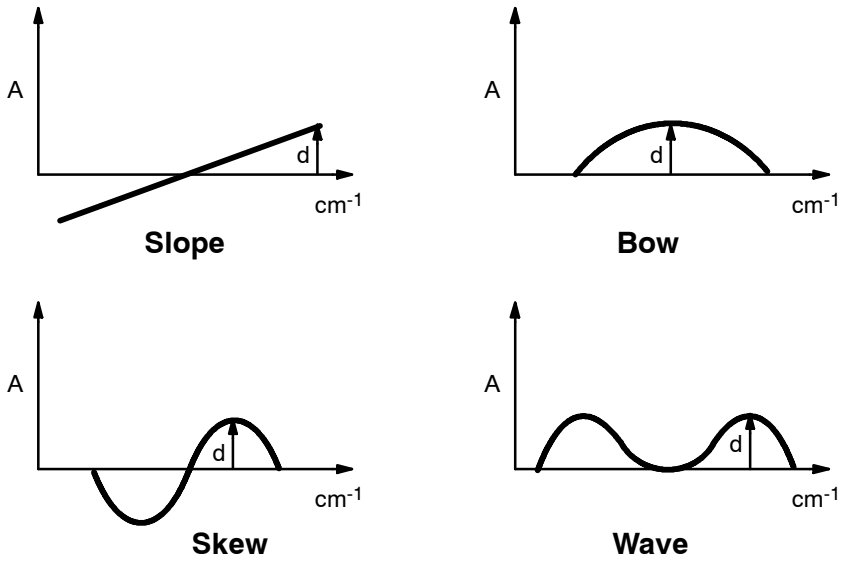


Figure 3-45 Four Orders of Baseline Correction

Baseline correction over a limited range

When the **range** Flat Option of Setup is at its factory setting, Flat, like the other processing commands, acts over the full range of the spectrum no matter what range is displayed.

However, if you change the **range** parameter in the Flat Options from **full** to **limited**, you can correct the baseline of only part of the spectrum, if you wish.

Setup options for Flat

The setup options for Flat are:

Flat #Terms Determines the number of orders of baseline correction that appear in the command line when you first press *flat*.

Flat Range Selects baseline correction over either the full range of the spectrum or a limited range (the range on the screen).

View Schange Switching off the scale change at 2000 cm^{-1} may help you to make judgments as you correct the baseline of the spectrum.

Setting the Flat Option in Setup Calc

1 At Ready For Next Command, press *setup* *OTHERS* *OTHERS* *calc*.
The Calculation Options screen appears.

2 Press *flat*.
The command line and soft keys in Figure 3-46 appear.

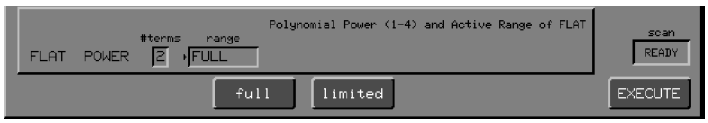


Figure 3-46 The Flat Option Command Line and Soft Keys

3 To change the number of fields in Flat, type a number (from 1 through 4) in the **#terms** field.

4 To change the range, press *full* or *limited*
or

To use the current range, press *EXECUTE*.

5 Press *EXIT*.
Ready For Next Command returns.

Using the Flat Command

Preparing to use Flat

To obtain good results with Flat, you must make sure that the relevant Setup options and the screen display are adjusted correctly for the baseline correction you want to do.

To set the Spectrum RXI so that you can interactively correct the baseline of a spectrum:

1 Make any necessary changes to the Setup options (see previous page).

2 Select the region that contains the spectrum that you want to correct.
The spectrum appears.

3 If the spectrum is displayed in %T, press **T/A**.
The spectrum appears in Absorbance.

Selecting the range for a limited-range flat

4 Using the horizontal arrow keys, display the part of the spectrum that you want to correct.

NOTE: *Limited-range flat executes over the range that is visible when you first enter a numeric value in the command line.*

Using Flat

5 Press **flat**.
The Flat command line and soft keys appear. The numeric fields are all zero, showing that no correction has taken place yet. If the Flat Range option is set to **limited***, the title over the command line includes* **(limited range)**.

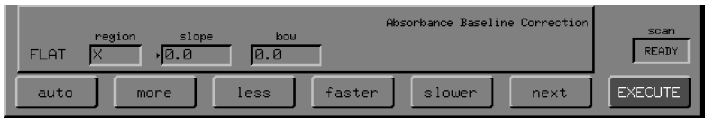


Figure 3-47 The Flat Command Line and Initial Soft Keys

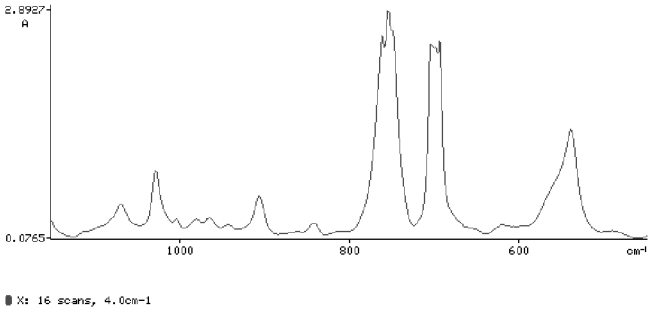


Figure 3-48 Selecting a Range to be Corrected

NOTE: *In Figure 3-48, only the portion of the spectrum from 1150 to 450 cm^{-1} is visible. A non-zero value has been entered in the* **slope** *field, so the view range is now the range to be corrected.*

If you want to, you can now adjust the view range to include more of the spectrum. The range over which Flat acts does not change.

Correcting the baseline

The following procedure assumes that the initial command line contained only the **slope** and **bow** fields.

1 If you want the baseline to be corrected automatically, go to step 13. Otherwise, steps 2 through 12 explain how to determine the four orders of baseline correction interactively.

2 Press ***hcursor***.
The horizontal cursor appears.

3 Adjust the slope until the two ends of the curve are at the same ordinate value, either by typing a value, or by using ***more***, ***less***, ***faster*** and ***slower*** to determine the appropriate slope interactively (Figure 3-49).
If you press ***enter*** *after typing a value, the spectrum is updated to show the effect of this amount of first-order correction, and the cursors move to the* **bow** *field.*

If you do not press ***enter*** *after typing a value, the cursors remain in the* **slope** *field, so you can type a different number or modify the slope using the soft keys.*

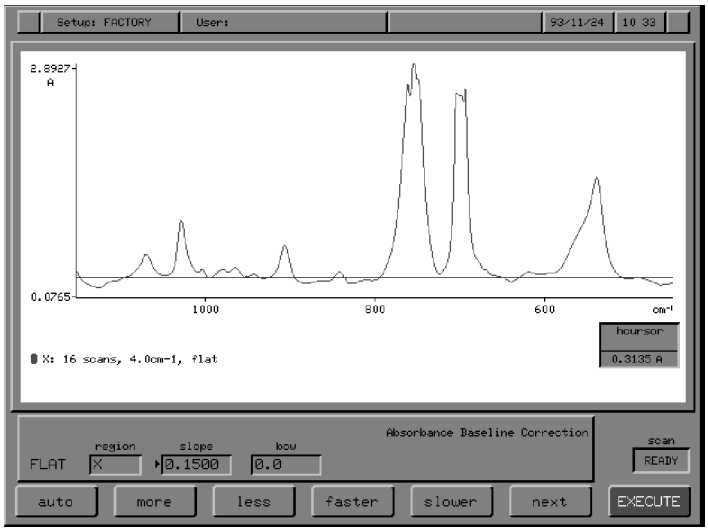


Figure 3-49 Correcting the Slope

4 When you are satisfied with the first-order correction, press (next) .
The cursors move to the **bow** *field.*

5 Eliminate the bow in a similar way to slope.

6 If you want to introduce a **skew** field, press shift (next) .
The cursors move to the **skew** *field.*

7 Eliminate the skew in a similar way to slope.

8 If you want to introduce a **wave** field, press shift (next) .
The cursors move to the **wave** *field.*

9 Eliminate the wave in a similar way to slope.

10 To return to the **slope** field, press enter .
The cursors return to the **slope** *field.*

11 If you want to *reduce* the number of orders of baseline correction, from the **wave** field press shift (next) .
Only the **slope** *field remains. The effects of other orders of baseline correction disappear from the spectrum.*

12 To modify your previous entries in the four fields, repeat steps 3 through 11.

13 If, at any point, you decide you want the baseline to be corrected automatically, press (auto).
The baseline of the spectrum is corrected, using whatever orders of correction are currently on the screen, and choosing suitable values for each. The resulting spectrum appears.

Executing the Flat Command

1 When you are satisfied with the appearance of the corrected spectrum, press EXECUTE.
The Flat command is executed over either the entire spectrum or a limited range, using the specified slope, bow, skew, and wave.

- *Ready For Next Command returns, with the corrected spectrum displayed.*
- *The word* **flat** *appears in the status line.*
- *The values of the numeric fields are placed with the status information for the spectrum and in the V-variables, beginning with V0.*

2 Restore the graphics display to the appearance you want:

* If you switched the scale change off in Setup, switch it back on now.
* If you changed the ordinate mode from %T to Absorbance, press T/A.
The spectrum returns to %T.

Height: Peak Height from Baseline

The height function reports the three results that are listed below and illustrated in Figure 3-50:

height The height of a peak from a baseline or from the horizontal axis.

width The full width at half height of the peak.

peak The exact wavenumber position of the peak.

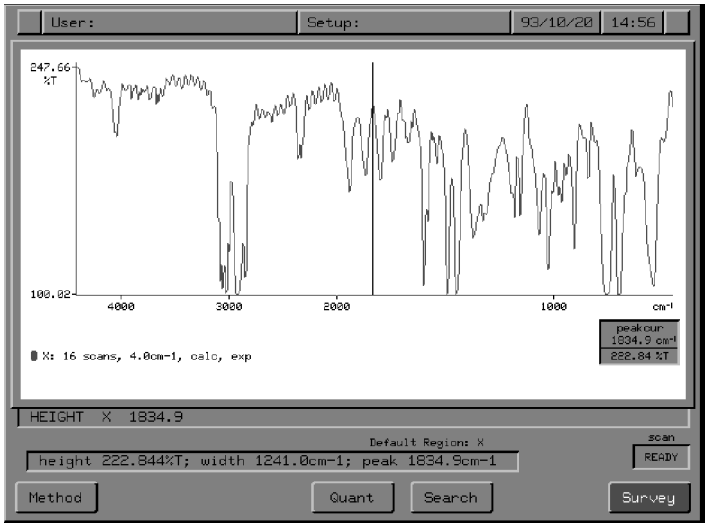


Figure 3-50 The Results of height

Specifying absorbance or transmittance height

The height function calculates the height of a peak either in absorbance or in transmittance, depending on the setting of **trans**.

- If the spectrum is displayed in absorbance, the height is calculated in absorbance
- If the spectrum is displayed in transmittance, the height is *still* calculated in absorbance unless **trans** is switched **on** (see page 3-98).

The title over the command line in the **height** user interaction tells you whether the height is calculated in transmittance or in absorbance.

You usually need the absorbance height even if your spectrum is displayed in transmittance. However, the transmittance height is useful in applications that involve filters or anti-reflection coatings.

Using height

1 At Ready For Next Command, press ***height***.
The command line and soft keys for height appear. The title over the command line tells you whether the height will be calculated in absorbance or in transmittance.

Figure 3-51 Command Line and Soft Keys for height

If more than one spectrum is displayed, all the spectra are removed except the spectrum in the default region.

2 If you want to calculate the height for a spectrum in a different region, press a region key.
The spectrum in the new region appears, and the new region is displayed in the **region** *field.*

3 If it is not already displayed, display the vertical cursor.

4 Position the vertical cursor approximately on the peak whose height you want to find, and press ***readcur***.
The approximate position of the peak appears in the **peak waveno** *field. Alternatively, you can just type the approximate position of the peak.*

5 Press ***enter***.
The cursor moves to the **base from** *field.*

NOTE: *Leave* **base from** *and* **base to** *empty if you want the peak height to the zero ordinate.*

Drawing a baseline

6 Move the vertical cursor to the first baseline point and press ***readcur***.
The wavenumber of this point appears in the **base from** *field*

7 Press **enter**.
A horizontal baseline through the **base from** *point appears (Figure 3-52), and the cursor moves to the* **base to** *field. The* **base to** *field contains the same number as the* **base from** *field because the baseline is currently horizontal. A tick on the horizontal axis marks the position of* **base from**.

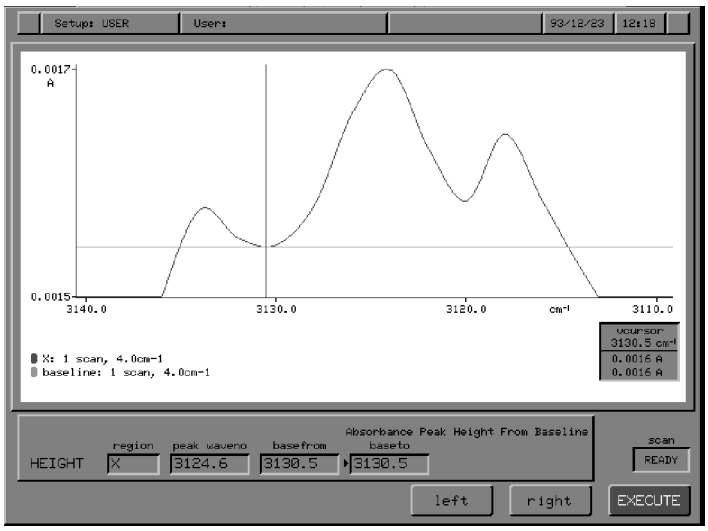


Figure 3-52 Horizontal Baseline Drawn by height

8 If you want to keep a horizontal baseline, use **left** and **right** to adjust the horizontal baseline to the exact position that you want.

Making the baseline slope

9 If you want a sloped baseline, move the vertical cursor to the second baseline point and press **readcur**.

10 Press **enter**.
The baseline now slopes so that it passes through both baseline points.

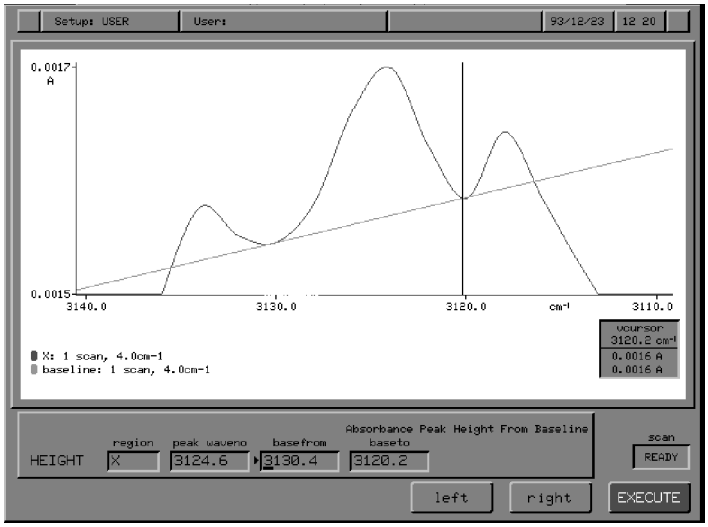


Figure 3-53 Slanted Baseline Drawn With height

11 Use (left) and (right) to adjust the sloped baseline.
[enter] *toggles the cursor between the* **base from** *field and the* **base to** *field. When the cursor is in the* **base from** *field,* (left) *and* (right) *move the first baseline point to the left or right along the spectrum; when the cursor is in the* **base to** *field,* (left) *and* (right) *move the second baseline point to the left or right along the spectrum.*

Executing height

12 When the screen display correctly represents the height you want to calculate, press (EXECUTE).
The baseline is removed from the spectrum.

Peak thresholds To find the peak position, **height** uses the peak threshold set in the View Peaks option of Setup. If no peak above the specified threshold is found within 20 cm^{-1} of the position you gave, the height at the given position is reported. When this happens, the **width** reported is zero, because there is no peak.

NOTE: *If your spectrum is displayed in transmittance, and* **trans** *is* **off**, *the peak threshold used by height is the absorbance peak threshold. If you set the threshold in transmittance, this value is not converted to absorbance – instead the previous absorbance threshold setting is used.*

Significant figures

If the peak whose height you are determining is very small, it may not be possible to display all the significant figures in a labelled result. To see the entire result, display the V-variables where the results are saved. For example, if you type **V0=**, the height saved in **V0** is displayed (the format of the results is determined by the **display** typed command, see *Advanced Operations*, Chapter 5, *Typed Commands*).

Layer: Thickness of Layer / Index of Layer

The layer function gives one of the following results, depending on the setting of the Calc Layer option of Setup.

- with Calc Layer set to **thick**, it gives the thickness of a layer (in μm)

or

- with Calc Layer set to **index**, it gives the refractive index of a layer

Layer calculates the thickness or the refractive index from spectral data, using the following equations:

$$t = \frac{10\,000\ m}{2(\nu_1 - \nu_2)\,(n^2 - \sin^2\theta)^{1/2}}$$

or

$$n = \sqrt{\frac{10\,000\ m}{2(t)\,(\nu_1 - \nu_2)} + \sin^2\theta}$$

where:

t	=	the thickness of the layer in μm.
ν_1 , ν_2	=	the wavenumber interval, in cm^{-1}, over which fringes in the spectrum are being counted. **Layer** uses the absolute value of this interval, so you can enter the two numbers in either order.
m	=	the number of fringes found in the wavenumber interval.
n	=	the refractive index of the material in the layer.
θ	=	the angle of incidence, in degrees, at which the spectrum was measured. The angle is measured relative to the normal to the surface.

Parallel-sided samples often produce spectra that have a sinusoidal variation in transmission. This variation is called a *fringe* or *channel spectrum* (Figure 3-54), and is caused by interference between the principal beam transmitted through the sample and a second beam caused by multiple reflection within the sample. Transmission is strongest when the extra optical path taken by the reflected beam is a multiple of the wavelength. If you know the spacing of the fringes and the refractive index of the sample, its thickness can be calculated; if you know the spacing and the thickness, its refractive index can be calculated.

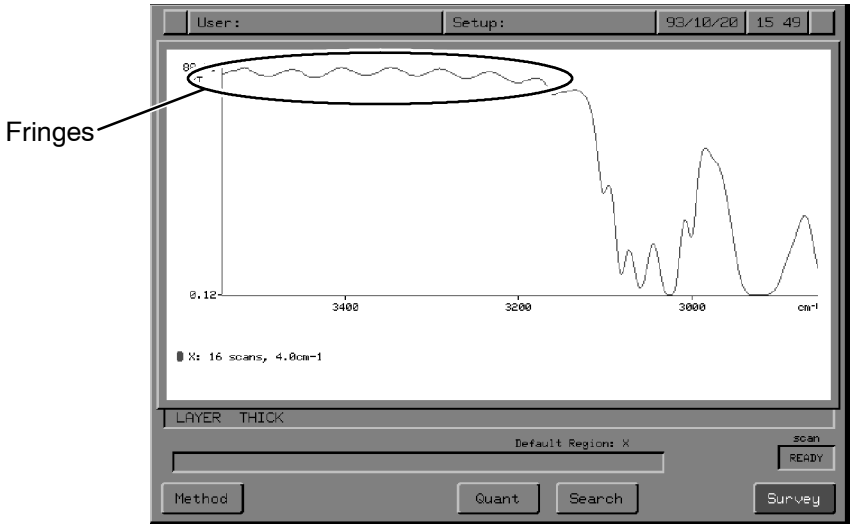


Figure 3-54 Fringes in the Spectrum of a Layer

Setting the layer option

1 At Ready For Next Command, press **setup** **OTHERS** **OTHERS** **calc** .
The Calculation options screen appears.

2 Press **layer** .
The command line and soft keys in Figure 3-55 appear.

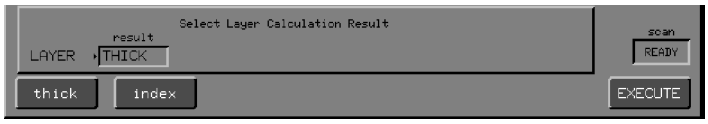


Figure 3-55 The Layer Option Command Line and Soft Keys

3 Change the setting by choosing an action key.
The Calculation options screen reappears.

4 Press EXIT .
Ready For Next Command returns.

Using layer

1 At Ready For Next Command, press layer .
If the **layer** *Calculation option of Setup is set to* **thick***, the command line and soft keys in Figure 3-56 appear. If* **layer** *is set to* **index***, the command line in Figure 3-57 appears.*

Figure 3-56 Command Line and Soft Keys for layer when it Calculates Thickness

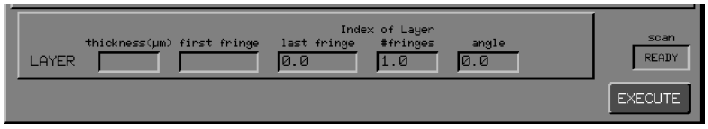


Figure 3-57 Command Line and Soft Keys for layer when it Calculates the Index of Refraction

2 In the first field of the command line, type either the index of refraction or the thickness of the layer, whichever is the prompt on your screen. Press enter .
The cursor moves to the **first fringe** *field.*

3 Enter the value in the **first fringe** field in either of the following ways:

a If you know the entire frequency interval, in wavenumbers, type it in the **first fringe** field. Press enter three times to keep the default settings of **last fringe** and **# fringes** fields at their default settings (**0.0** and **1.0**, respectively).
The cursor moves to the **angle of incidence** *field.*

b Go to step 4, or, if the angle of incidence is 0, go to step 5.

or

a Type the wavenumber position of the first fringe, or enter it from the spectrum with **readcur**. Press **enter**.
The cursor moves to the **last fringe** *field.*

b Type the position of the last fringe, or enter it with **readcur**. Press **enter**.
The cursor moves to the **# fringes** *field.*

c Type the number of fringes that occur in the frequency interval. Press **enter**.
The cursor moves to the **angle of incidence** *field.*

4 Type the angle of incidence (in degrees) at which the spectrum was measured.

5 Press EXECUTE.
The calculator computes the thickness or the refractive index of the layer, places it in **V0**, *and reports it on the Command line as shown in Figures 3-58 and 3-59.*

Ready For Next Command returns.

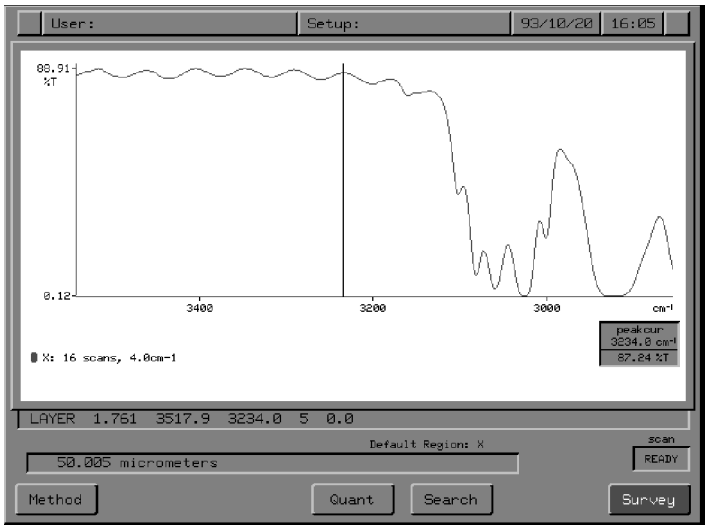


Figure 3-58 Result of Calculating the Thickness of a Layer

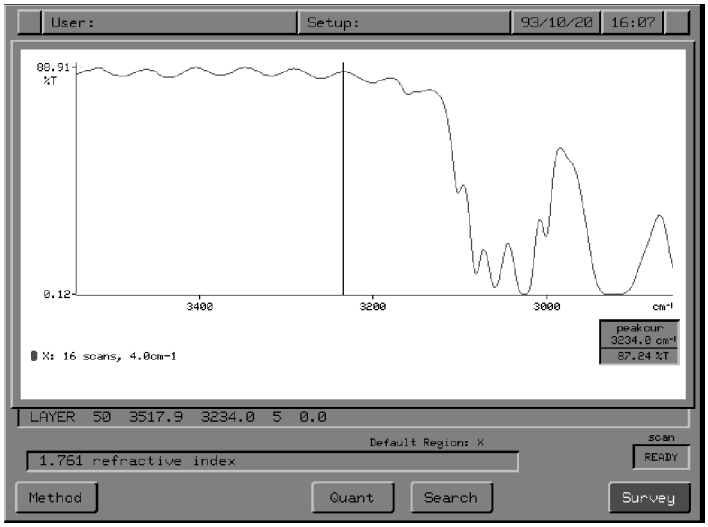


Figure 3-59 Result of Calculating the Index of Refraction of a Layer

Using layer in expressions

If the Layer Calculation option of Setup is set to **thick**, use the first format; if it is set to **index**, use the second.

Format	Examples
layer(n,ν_1,ν_2,m,θ)=	layer(1,3850,1480,9,0)
layer(t,ν_1,ν_2,m,θ)=	layer(20,3850,1480,9,0)

where:

t = the thickness of the layer in μm.

$\nu_1 - \nu_2$ = the wavenumber interval, in cm^{-1}, over which fringes in the spectrum are being counted (Figure 3-54). **Layer** uses the absolute value of this interval, so the two numbers can be entered in either order.

m = the number of fringes found in the wavenumber interval.

n = the refractive index of the material in the layer.

θ = the angle of incidence, in degrees, at which the spectrum was measured. The angle is measured relative to the normal to the surface.

Micron: Micron/Wavenumber Conversion

This function gives only one result – the number of microns corresponding to a specified number of wavenumbers, or vice versa. It uses the relationship:

wavenumber × micron = 10 000

1 At Ready For Next Command, press **micron**.
The command line and soft keys in Figure 3-60 appear. The alphanumeric cursor is in the **number** *field.*

Figure 3-60 Command Line and Soft Keys for micron

2 Type a number.

3 Press **EXECUTE**.
The result appears on the Command line. It is assigned to variable **V0**.

Ready For Next Command returns.

Reverse Entry

Format	Example
n micron	2570 micron

Using micron in expressions

Format	Examples
micron(n)=	micron(4300)=
	micron(V7-300)=

where n is a positive number.

Smooth: Reducing Noise by Smoothing a Spectrum

Smoothing is used to reduce the noise level in a spectrum. When smoothing is applied, the bands in the spectrum are broadened, and the effect is greatest on the narrowest features, usually the baseline noise. Thus it may be possible to obtain a useful reduction in the amplitude of the noise before the spectral features are broadened so much that information is lost. The amount of distortion introduced by smoothing can be estimated by subtracting the smoothed spectrum from the original. Alternatives to smoothing which should be considered are to accumulate more scans or to use lower resolution.

About smooth

The Smooth command specifies a band width, the *smoothing width*, above which you want no loss of resolution (that is, no broadening of bands).

The upper limit of the smoothing width must be determined separately for each spectrum. Do not use a smoothing width (w) that exceeds the width of the narrowest band of interest in the spectrum, measured at half its height (h in Figure 3-61). Above this width, loss of detail occurs rapidly.

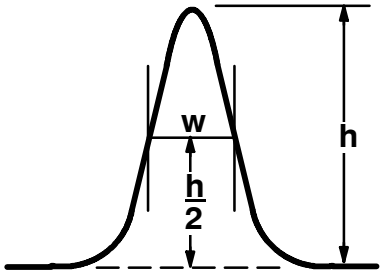


Figure 3-61 Defining the Smoothing Width

When you specify a smoothing width, a noise reduction factor, called *improvement*, is calculated; improvement is the reciprocal of the fractional noise remaining. For example, if the noise is reduced by one quarter, the noise remaining is three quarters. The noise reduction factor (improvement) is $^4/_3$, or 1.33.

When the Smooth command executes, the values for the smoothing width and the improvement are placed with the status information for the spectrum and in V-variables V0 and V1, respectively.

Using the Smooth Command

Determining the upper limit of the smoothing width

1 Before you access Smooth, determine the upper limit of the smoothing width for your spectrum:

a If the spectrum is in %T, press **T/A**.
The spectrum appears in Absorbance.

b At Ready For Next Command, press **vcursor**.
The vertical cursor appears.

c Move the cursor to the narrowest significant band in the spectrum, or to a very narrow band.

d Use **< >** to expand the spectrum horizontally until the narrow band is clearly displayed.

e Move the cursor to the point on the left-hand side of the band where the band is approximately half its full height (Figure 3-62).

f Press **readcur** **-**.
The command line is similar to Figure 3-62.

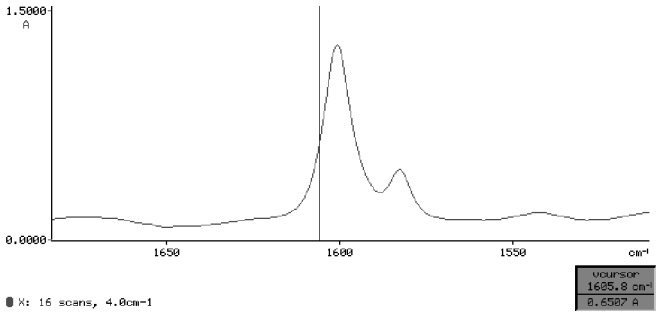


Figure 3-62 Determining the Band Width at Half Height

g Move the cursor to the point on the right-hand side of the band where the band is approximately half its full height.

h Press ***readcur*** [=].
The two wavenumbers are subtracted, and the result is the band width at half height. Do not use a smoothing width that is greater than this value.

i Press ***rerange***.
The display returns to its default range.

2 Press ***smooth***.
The command line and soft keys in Figure 3-63 appear. The **improvement** *field is* **1.0000***, showing that no smoothing has taken place yet.*

Figure 3-63 The Smooth Command Line and Initial Soft Keys

3 Specify the smoothing width in either of the following ways, keeping it below the limit you determined in step 1.

* Type a width and press ***enter***.
The spectrum is updated to show the effect of smoothing, and **improvement** *is updated. You can then type a different number, or you can adjust the width using the soft keys, as described below.*

* Use ***more***, ***less***, ***faster*** and ***slower*** to determine the appropriate smoothing width interactively.

4 Press ***EXECUTE***.
The Smooth command is executed, using the specified smoothing width. When the computation is complete:

- *Ready For Next Command returns, with the improvement reported in the Command line and the smoothed spectrum displayed.*
- *The status line includes the word* **smooth**.
- *The values for the smoothing width and the improvement are placed with the status information for the spectrum and in V-variables V0 and V1, respectively.*

T/A: Switching the Ordinate Mode betweenTransmittance and Absorbance

In many respects, transmittance is the *natural* ordinate scale of the spectrometer. The instrument responds linearly to energy falling on the detector, and transmittance is simply the ratio of the energy in the presence of the sample to the energy without the sample. On this *energy-linear* scale, the noise (inevitably generated by the detector) is largely independent of the energy, so that a small difference in transmittance near 0%T is just as significant as a similar difference near 100%T.

Unfortunately, in this *natural* scale, transmittances are multiplicative rather than additive. For example, double the thickness or the concentration of the sample and what was 50%T becomes 25%T; 10%T becomes 1%T; and 1%T becomes 0.01%T, almost immeasurably small. In transmittance, as the concentration or thickness increases, strongly absorbing bands apparently change their shape as they start to *bottom out* near 0%T. An example of this effect can be seen quite clearly in the demonstration of the Abex command (page 3-53).

This non-additive, non-linear behaviour of spectra can be fixed quite easily by converting to the logarithmic ordinate scale of absorbance. In absorbance, the multiplications become additions; doubling the thickness or concentration simply doubles the absorbance and the shape of the spectrum stays substantially the same.

The absorbance scale seems much more appropriate to absorption spectroscopy but nevertheless has a few drawbacks, for example, 0%T on this scale converts to an infinite absorbance value. As a result, strongly absorbing features become huge in absorbance and are also correspondingly noisy because small changes of transmittance near 0%T have a much larger effect on the absorbance than similar changes near 100%T. Visually, the large absorbance peaks with their (perhaps not obviously) noisy tops dominate the display, while important detail near the baseline gets overlooked.

With these disadvantages in mind, a transmittance scale may in practice be preferable for display purposes, particularly when the range of concentration and thickness of samples is fairly limited.

From the Spectrum RXI's point of view, the choice of ordinate scale is not normally significant, because the major functions all contain the arithmetic necessary to convert to the ordinate scale appropriate to the calculation. An exception is direct arithmetic on spectra using the calculator where the result will depend upon the current display mode. For example, X + Y added in transmittance gives a result different from the same operation in absorbance mode.

About T/A

Pressing **T/A** toggles the ordinate mode of displayed spectra between percent transmittance (%T) and absorbance (A) units; the display changes immediately. Figure 3-64 shows a spectrum in %T. Figure 3-65 shows the same spectrum after **T/A** was pressed.

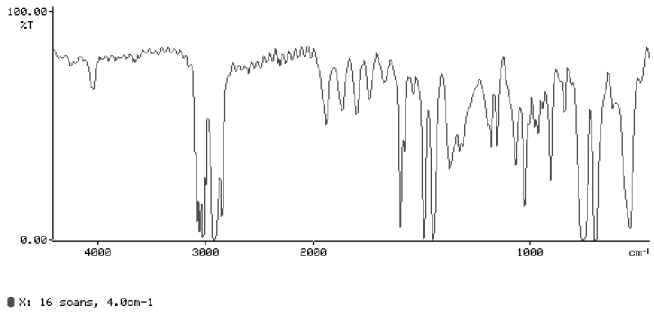


Figure 3-64 A Spectrum in the %T Ordinate Mode

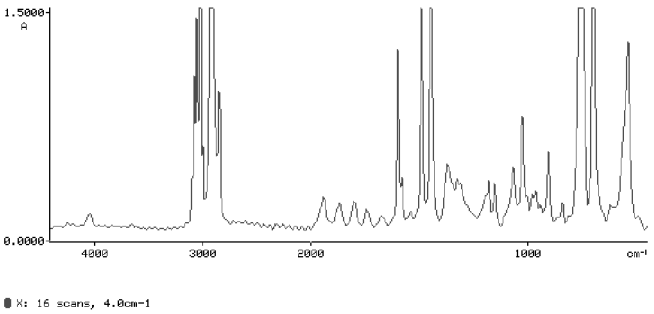


Figure 3-65 The Spectrum from Figure 3-64 Displayed in Absorbance

Often you can decide to work consistently in either transmittance or absorbance, hence changing the ordinate display mode affects not only the spectrum that is currently displayed, but also other spectra of the same type. That is, if the display is a ratio spectrum, other ratio spectra are affected too.

- All spectra of the same type that are subsequently displayed are shown in the new ordinate mode.
- Data of the same type that are subsequently collected with **scan** are in the new ordinate mode.
- Spectra of the same type stored on disk are displayed in the new ordinate mode when they are retrieved, irrespective of the ordinate mode of the stored data.
- Data in memory remain in their original mode until processing commands make conversion necessary.
- Data stored on disk are not converted, even though they are displayed in the new mode when retrieved.
- **T/A** has no effect when an interferogram is displayed.

Processing Data in Transmittance

For most applications, many of the Process commands and the **height** and **area** calculator functions perform their calculations in absorbance, whether the displayed spectrum is in absorbance or %T.

However, if you are working with emission spectra, filters, or anti-reflection coatings, you may want to process data in transmittance. The **trans** Calculation Option enables you to set the Spectrum RXI to do this.

- If **trans** is switched off (the factory default setting), calculations are performed in absorbance whatever the units of the displayed spectrum.
- If **trans** is switched on, calculations are performed in absorbance if the current ordinate mode is A, or in transmittance if the ordinate mode is %T.

If you only want to switch **trans** on for certain, specific commands, use the selection numbers in Table 3-12 rather than the words **ON** and **OFF**. To select one command to be performed in transmittance, enter its selection number in the **trans** command line. To select more than one command, enter the *sum* of their selection numbers.

Selection Number	Command for which Transmittance is Switched On
0 or **OFF**	None
1	**Area**
2	**Compare**
16	**Diff**
32	**Flat**
64	**Height**
128	**Peak**, the Peaks cursor, peak location in **Height**, **Mark**
255 or **ON**	All the above commands.

Table 3-12 Selecting Commands to be Calculated in Transmittance

The title lines of commands affected by this option always tell you whether the calculation will be performed in absorbance or transmittance.

Switching transmittance calculation on or off

1 At Ready For Next Command, press
setup *OTHERS* *OTHERS* *calc* *trans* .
The command line and soft keys shown in Figure 3-66 appear.

Figure 3-66 The Trans Option Command Line and Soft Keys

2 Switch **trans** *on* or *off* .

or

Type the sum of the selection numbers of the commands that you want to be calculated in absorbance (see Table 3-12 for the selection numbers).

or

Select the current setting by pressing *EXECUTE* .

3 Press *EXIT* .
Ready For Next Command returns.

Printing and Plotting 4

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Introduction to Plotting

You can customize the plotting of spectra or interferograms to meet the requirements of your laboratory. Plotting is a *detached* operation, so, while the plotter is busy, you can use the keypad for other tasks.

Before you can use a plotter connected to the Spectrum RXI, you must configure the Spectrum RXI for that plotter (see *Configuring the Spectrum RXI for Peripheral Devices* in *Communicating with Other Devices* in *Advanced Operations*).

NOTE: *The following devices support HPGL, and can therefore be used as a printer or a plotter: HP LaserJet III, HP LaserJet IV and Paintjet 1200.*

NOTE: *Note that some Plot Options must be set differently for LaserJets and Desk Jets. This is because LaserJets have more memory, so the page is set up before it is printed, but Desk Jets print as they receive information. Therefore, if you have created a method that includes plotting to one of these types of printer, the printout will be different if you connect the other type of printer. For information about setting the position of the plot for these printers, see page 4-26.*

NOTE: *If you are plotting to a Desk Jet Printer or a PCL5 Printer, there is more information about setting up the printer* (see *Configuring the Spectrum RXI for Peripheral Devices* in *Communicating with Other Devices* in *Advanced Operations*).

Components of a Plot

Unless you choose other Setup options, the plot consists of the components described below and shown in Figure 4-1.

Component	Description
Data	There can be up to three spectra or interferograms on each plot.
Axes and their labels	The ordinate axis is at the left-hand edge of the plot window; the abscissa axis is at the bottom. The Plot Window option in Setup sets the size and position of the axes on the paper.
Cursor	If a graphics cursor is displayed on the screen, the cursor and its annotation are plotted.
Caption	The caption is plotted at the bottom of the paper (see the Annotation Window in Figure 4-1). When a plot contains one spectrum, the caption has three lines; if the plot contains more than one spectrum, there is a one-line caption for each spectrum. (The content of the caption is described on page 4-11.)

More Than One Plot on a Page

If you want more than one plot on the same page, leave the same sheet of paper in the plotter. (If the Plot Advance option is on, switch it off.)

- To put the next plot in a different position, change the setting of the Plot Window option.
- To overlay the plots, do not change Plot Window.

Make sure you either switch off the captions for all but one plot or change the position of successive captions, so they do not overwrite each other. Use the Plot Caption option in Setup for this (see *Plotting a Caption* on page 4-11).

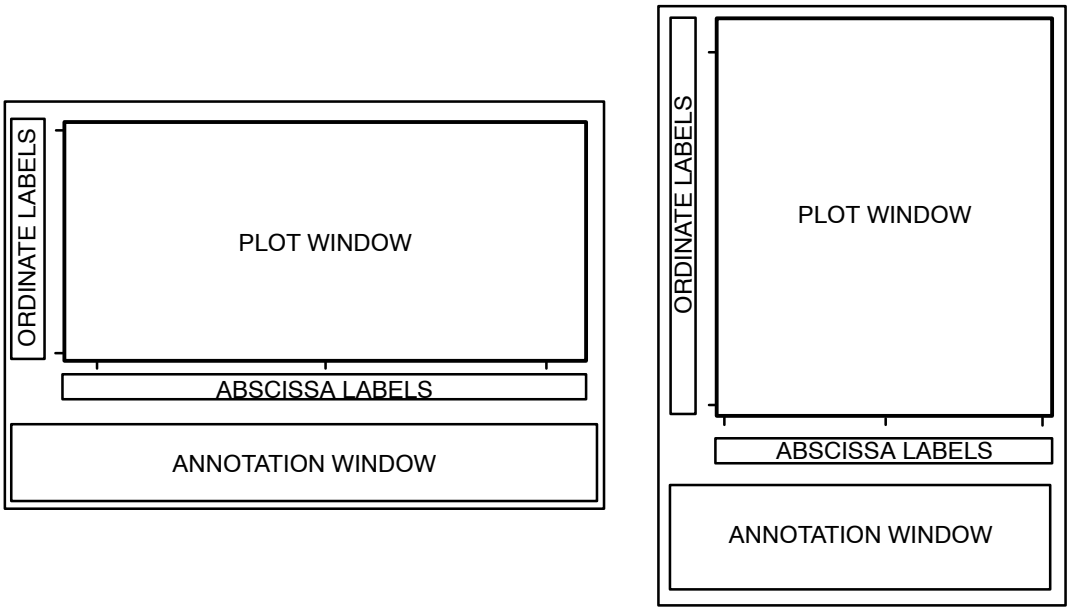

Figure 4-1 Format of a Single Plot

Using Various Kinds of Paper

The Plot Paper option of Setup enables you to choose plain paper or graph paper; either sheets or rolls of paper can be used.

Note the following when you use various kinds of paper for plotting:

graph paper	Use the Plot Paper option to test the alignment of the plotter pen with the origin. The Plot command plots the ordinate and abscissa ranges that are on the screen; the position of the plot is set using the Plot Window options. Therefore, you can make the scaling of the plot match the grid on the paper by changing either the Plot Window options or the displayed spectrum.
chart paper	When you select **chart** in Plot Paper, the Plot options are set appropriately for Perkin-Elmer chart paper. You can still use the **Pens**, **Line**, **Advance**, and **Peaks** options.

NOTE: *The default settings assume a paper size of 10 inches x 8 inches (US Letter size). To use a larger sheet of paper, use the Plot Window option to set the paper size.*

Setting up the Plot Options

The Plot Options

The Plot Options define how the components of the plot are arranged on the paper. The Plot Options are described on the following pages, and are summarized below:

Option	Function	Page
absc(issa)	Sets the abscissa units (cm^{-1} or microns).	4-8
advance	Before each plot, automatically feeds the next sheet of paper to the plotter.	4-9
axes	Switches the plotting of axes on and off.	4-10
caption	Switches the plotting of captions on and off, and sets their position.	4-11
grid	Enables you to plot a grid on plain paper	4-13
lines	Sets the type of line used to plot each spectrum.	4-14
paper	Sets the type of paper being used in the plotter. Aligns the pen, if necessary.	4-15
peaks	Enables you to label peaks in plotted spectra.	4-19
pens	Defines the color in which each plot component is plotted.	4-21
quality	Enables you to print a *draft* quality spectrum.	4-22
rotate	Rotates the plot on the paper 90 degrees counter-clockwise from its usual position.	4-23
window	Sets the size and position of the axes on which the spectra are plotted.	4-24

Table 4-1 Plot Options

Displaying the Plot Options

1 At Ready For Next Command, press **setup** (plot).
The table and soft keys shown in Figure 4-2 appear. The table shows the factory default values for the Plot options that are currently displayed; press (OTHERS) *to see another set of Plot option soft keys (Figure 4-3). Press* (OTHERS) *again to see the final Plot options (Figure 4-4).*

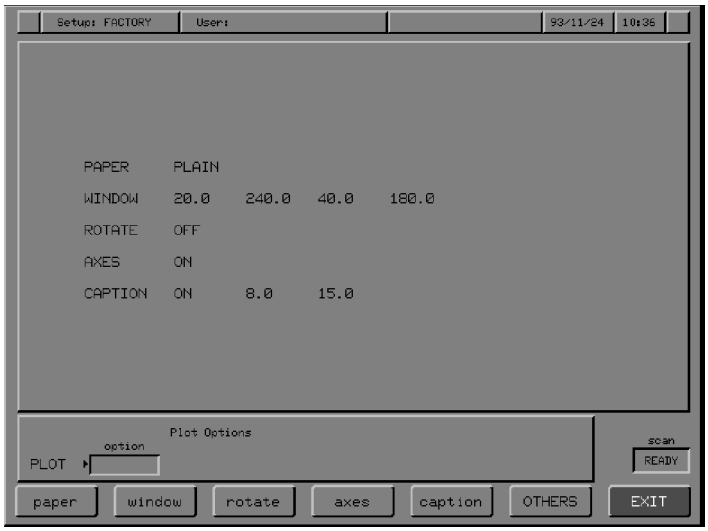

Figure 4-2 The First Plot Options Screen

Figure 4-3 The Second Plot Options Screen

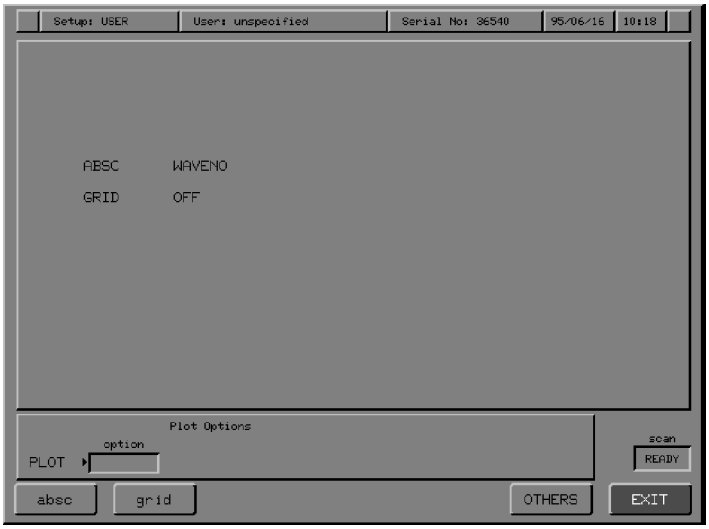

Figure 4-4 The Third Plot Options Screen

Choosing the Abscissa Units

Conventionally, mid-infrared spectra are presented on an abscissa linear in wavenumber. This is particularly appropriate for FT-IR instruments because Fourier transformation generates data that are evenly spaced in wavenumbers. However, for historical reasons, or for compatibility with other types of spectroscopy, it may be appropriate to display the data on a linear wavelength scale.

Although the abscissa units for spectra displayed on the screen are always wavenumbers, you can choose either wavenumbers or microns as the abscissa units for plots. (Interferograms are *always* plotted in microns.)

1 At Ready For Next Command, press **setup** **plot** **OTHERS** **OTHERS** **absc** .
The command line and soft keys in Figure 4-5 are displayed.

Figure 4-5 The Plot Absc Command Line and Soft Keys

2 Choose an option.

3 Press **EXECUTE** **EXIT** .
Ready For Next Command returns.

NOTE: *If you choose* **micron** *and the Plot Axes option is on, a second abscissa scale across the top of the plot shows the wavenumbers (Figure 4-6). Micron plots do not have a scale change (see* Schange *on page 3-12).*

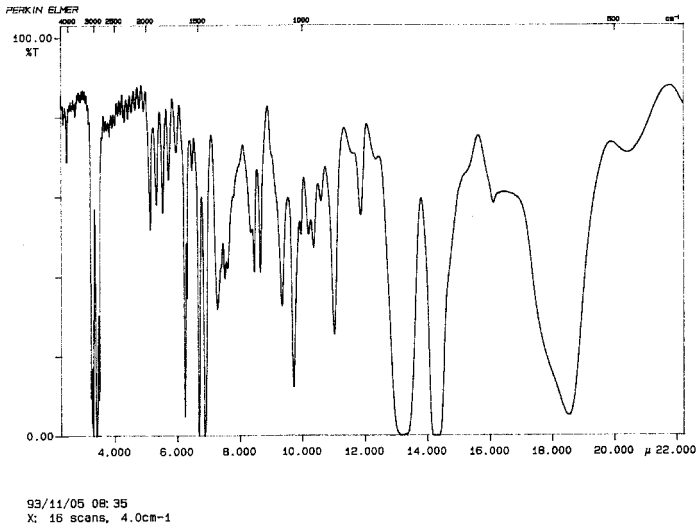

Figure 4-6 Plot with Microns as the Abscissa Units

Overlaying Plots and Plot Advance

When Plot Advance is on (the factory default setting), a new sheet of paper is fed to the plotter at the beginning of each plot, if your plotter can do this; if it cannot, nothing happens.

To overlay plots, switch Plot Advance off so that the same paper is used again.

NOTE: *To overlay plots on a LaserJet or DeskJet, set advance to off for all except the last plot so that a new sheet of paper is fed to the plotter after the last plot.*

1 At Ready For Next Command, press **setup** **plot** **OTHERS** **advance** .
The command line and soft keys in Figure 4-7 are displayed.

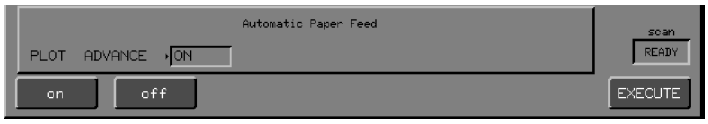

Figure 4-7 The Plot Advance Command Line and Soft Keys

2 Choose a setting.

3 Press **EXECUTE** **EXIT** .
Ready For Next Command returns.

Plotting Axes

You can switch the plotting of either or both of the axes on or off; axes include the axis lines themselves, the tick marks, the numbers, and the units label. The Plot Axes settings are:

on plots both axes. (This is the factory default.)

off plots neither axis.

x only plots only the horizontal axis.

y only plots only the vertical axis.

When you want to overlay plots, plot the axes only once then choose Plot Axes **off**.

1 At Ready For Next Command, press **setup** **plot** **axes**.
The command line and soft keys in Figure 4-8 are displayed.

Figure 4-8 The Plot Axes Command Line and Soft Keys

2 Choose one of the settings.

3 Press **EXECUTE** **EXIT**.
Ready For Next Command returns.

Plotting a Caption

The caption is the annotation plotted below the plot window. You can change the content and the position of the caption.

Content of the caption

When Plot Caption is **on** and you are plotting only one spectrum, there are three lines of information below the plot window:

line 1	the date and time when the spectrum was collected, and the name of the user.
line 2	the filename or the spectrum region where the spectrum is stored, and the conditions under which it was collected.
line 3	a comment line, if you have attached one to the spectrum.

If the plot contains two or three spectra, the caption is shorter; each spectrum has a one-line title containing:

the filename or spectrum region;

the comment, if any, or the conditions;

the date the spectrum was obtained.

Settings of Plot Caption

The Plot Caption option settings are:

on	full annotation for one spectrum, a shortened annotation for two or three spectra, as described above. (This is the factory default.)
comment	only the comment is plotted for each spectrum. If there is no comment, the line is blank.
off	no caption. You must switch Plot Caption off (or move the caption) when there are several plots on the same sheet of paper; otherwise, the first set of captions is overwritten.
reset	restores the factory default settings (caption on, located at the default position).

Position of the caption

You can choose the x and y coordinates of the first character of the caption. The coordinates are measured in millimeters from the bottom left-hand corner of the paper. If the caption is more than one line long, successive lines begin directly under the first x,y position.

If you change the default position, make sure that the caption still fits on the paper.

Setting Plot Caption

1 At Ready For Next Command, press **setup** (plot) (caption) .
The command line and soft keys in Figure 4-9 are displayed.

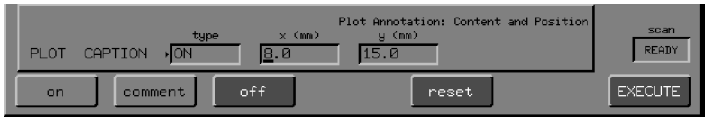

Figure 4-9 The Plot Caption Command Line and Soft Keys

2 Choose the option you require.
One of the following happens:

If you pressed an action key, the command executes and the first Plot options screen returns.

If you pressed **on** *or* **comment***, the* **type** *field changes. The soft keys remain. The cursor is in the* **x** *field.*

3 If you do not want to change the position of the caption, go to step 5. Otherwise, type the horizontal distance (in mm) of the first character of the caption from the bottom left-hand corner of the paper. Press **enter**.
The cursor moves to the **y** *field.*

4 Type the vertical distance of the first character from the bottom left-hand corner of the paper.

5 Press EXECUTE EXIT .
Ready For Next Command returns.

Adding a Grid to Plots

The **plot grid** command enables you to add a grid to a plot. The command is only available if you have set **plot paper** to **plain**.

1 At Ready For Next Command, press
setup (plot) (OTHERS) (OTHERS) (grid) .
The Plot Grid command line and soft keys appear.

Figure 4-10 The Plot Grid Command Line and Soft Keys

2 Press the key you require:

off switches the grid off;

auto switches the grid on. The grid spacing is generated by the Spectrum RXI;

on switches the grid on. You specify the x and y grid spacing using the units set in **plot absc**. The minimum grid spacing that will plot is 1 mm. If the grid increment is so narrow that grid lines are less than 1 mm apart, the increment is doubled until they are more than 1 mm apart.

NOTE: *If you set* **incr** *to* **0***, then the grid component is switched off – that is,* **plot grid on 0 0** *is equivalent to* **plot grid off**.
plot grid on 100 0 *plots only abscissa lines every 100 cm^{-1}.*
If you set **incr** *to* **–1***, then the grid is generated automatically – that is,* **plot grid on –1 –1** *is equivalent to* **plot grid auto**.
We recommend that you use **plot grid auto***, which gives the best results in most situations, and that you set the pen width to 0.3 to prevent the grid dominating.*

3 Press *EXECUTE* *EXIT* .
Ready For Next Command returns.

Plotting Spectra using Different Line Types

Dotted and dashed lines

A plot can contain up to three spectra. If your plotter has more than one pen, you usually distinguish the spectra by color. However, if your plotter has only one pen, or if you are going to photocopy the plots, you can use a different line type for each spectrum.

Three line types are provided, and the factory default settings are:

spectrum 1 solid;

spectrum 2 dashes and dots;

spectrum 3 dashes.

However, you can set each spectrum for whichever line type you want, or make them all the same.

Line width

If you are plotting to a LaserJet or Desk Jet, you can also set the width of the lines: from 0.1 mm to 0.9 mm, in steps of 0.1 mm. If you are plotting an unexpanded spectrum with fine detail, use a narrow line so that the detail appears clearly on the plot. If you are preparing a plot for publication or transfer to a slide, use a wide line so that the plot can be reproduced clearly.

Line styles for the grid

If you have **plot grid** switched on, you can set the line type and width for the grid. We recommend that you choose the line style **dotted**, which is only available for the grid. Using **dotted** for the grid line style increases the lifetime of the cartridge and also reduces the dominance of the grid in the final plot.

Setting the line type

1 At Ready For Next Command, press *setup* *plot* *OTHERS* *lines*.
The command line and soft keys in Figure 4-11 appear. The soft key cursor is in the **spectrum 1** *field.*

Figure 4-11 The Plot Lines Command Line and Soft Keys

2 Choose the line type for spectrum 1.
The cursor moves to the **spectrum 2** *field.*

3 Choose the line type for spectrum 2 and spectrum 3.
If you have **plot grid** *switched on, the cursor moves to the* **grid** *field; otherwise, the cursor moves to the* **width** *field.*

4 Choose the line style for the grid, if necessary.
The cursor moves to the **width** *field.*

5 Type the width of the line, in mm, in the **width** field.
The width must be between 0.1 mm and 0.9 mm, in steps of 0.1 mm.

6 Press EXECUTE EXIT .
Ready For Next Command returns.

Setting the Paper Type

You can use three different kinds of paper for plotting:

plain	sheets of paper. (This is the factory default.)
chart	preprinted sheets supplied by Perkin-Elmer. These contain labelled axes, a gridded plot window, and labelled lines where you can write annotations.
graph	sheets of graph paper.

The following pages give the procedures for:

- choosing the type of paper;
- aligning the plotter pen with chart paper and with graph paper.

Choosing the type of paper

1 At Ready For Next Command, press setup plot paper .
If the current paper type is **plain***, the soft keys shown in Figure 4-12 appear.*

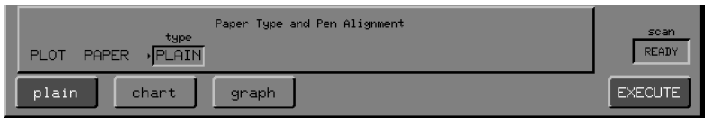

Figure 4-12 The Plot Paper Soft Keys when the Paper Type is plain

If the current paper type is **chart** *or* **graph***, the soft keys are similar to Figure 4-13.*

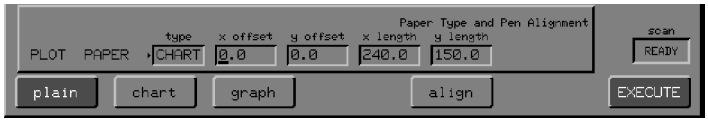

Figure 4-13 The Plot Paper Soft Keys when the Paper Type is graph or chart

2 If you do not want to use the current paper type, choose one of the others. *One of the following happens:*

If you chose **plain***, the command executes and the first Plot Options screen returns.*

If you chose **chart** *or* **graph***, the soft keys for aligning the pen appear.*

3 If the paper type is correct and you only want to align the plotter pen, press ***align***.
The soft keys for aligning the pen appear.

Aligning the pen with the chart paper

When you use Perkin-Elmer chart paper, you must align the pen with two points: the origin and the top right-hand corner of the plot window:

- **x offset** and **y offset** correct the initial position of the pen so that the pen lies over the origin on the chart paper.
- **x length** and **y length** correct the pen position when the pen is at the top right-hand corner of the paper, so that it lies over the top right-hand corner of the chart.

Two alignment marks are printed on the graph paper, to confirm that it is aligned correctly.

When you begin the alignment procedure, the command line and soft keys are similar to Figure 4-14. To align the pen with the chart paper, follow steps 1 through 6 on page 4-17.

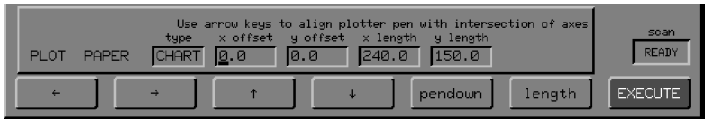

Figure 4-14 Command Line and Soft Keys for Aligning the Pen with Chart Paper

Aligning the pen with graph paper

When you select **graph** as the paper type, soft keys appear that enable you to align the plotter pen with the origin on the graph paper (Figure 4-15). The pen is initially at the bottom left-hand corner of the plot window that is defined by the Plot Window option. To align the pen with the graph paper, follow steps 1, 2 and 6 below.

Figure 4-15 Command Line and Soft Keys for Aligning the Pen with Graph Paper

1 Align the pen with the origin on the paper in either of the following ways:

Alignment using soft keys

a Using the horizontal arrow soft keys, move the pen left and right until it is aligned with the origin on the paper. Press ***enter***.
Either the **x offset** *or the* **y offset** *changes, depending on the setting of Plot Rotate.*

b Using the vertical arrow soft keys, move the pen up and down until it is above the origin. Press ***enter***.
The other offset changes.

Alignment using typed offsets

a Type a number of millimeters in the **x offset** field. Press ***enter***.
The pen moves to an abscissa position the specified distance from the expected origin. The cursor moves to the **y offset** *field.*

b Type a number of millimeters in the **y offset** field. Press ***enter***.
The pen moves to an ordinate position the specified distance from the expected origin. The cursor returns to the **x offset** *field.*

c Repeat steps a and b until the pen is above the origin.

2 Press (pendown).
The pen makes a dot on the paper. If you are using chart paper, the pen stays down until you release the soft key. If you are using graph paper, the pen stays down until you press (penup).

If the dot is not at the origin, repeat steps 1 and 2.

If you are using graph paper, go to step 6 now.

3 When the pen is aligned with the origin, press (length).
The pen moves to the expected position at the top right-hand corner of the plot window, and the cursor moves to the **x length** *field.*

4 Using either the arrow soft keys or typed distances, align the pen with the top right-hand corner of the plot window in the same way.

5 Press (pendown).
The pen makes a dot on the paper. If the dot is not at the top right-hand corner of the plot window, repeat steps 4 and 5.

6 When the pen is correctly aligned with both the origin and the top right-hand corner, press (EXECUTE) (EXIT).
The Plot Paper command executes. Ready For Next Command returns, and the pen moves to the origin.

Labelling Peaks on a Plot

You can choose the method that is used to select the peaks that are labelled (automatic or manual), and the content of the peak labels. You never see labels on the screen, only on plots. Figure 4-16 shows a plot with seven labelled peaks; the abscissa values are plotted.

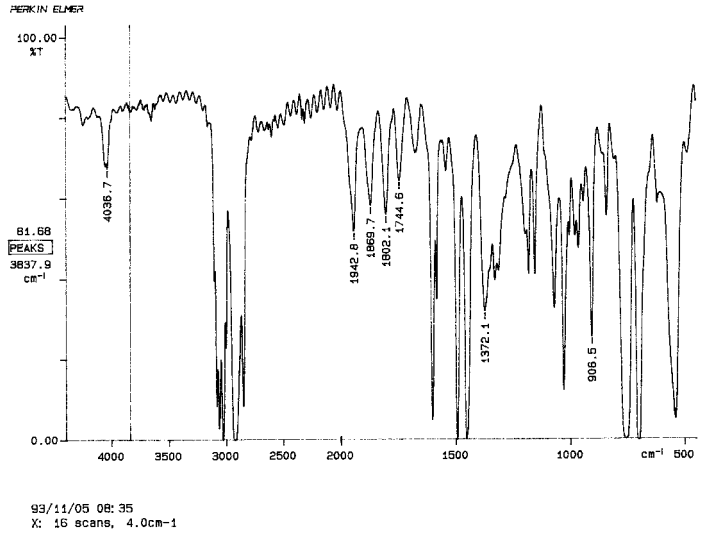

Figure 4-16 A Plot with Labelled Peaks

Only plots of one spectrum can be labelled; if you want to label a plot of two or three spectra, plot them individually, overlaid on the same paper.

Peak selection The positions to be labelled on the plot can be chosen in either or both of two ways:

- **automatic selection** – The peaks that would be listed in a peak table are labelled (threshold set by Setup View Peaks), and you can also manually select other peaks.
- **manual selection** – You use the vertical cursor and the ***mark*** key to mark the positions that you want to label. These marks, but not the labels, appear on the screen (***mark*** is described in *Marking a Spectrum for Labelling*, starting on page 3-36). This is the factory default setting.

Content of the peak labels

Peaks can be labelled with their abscissa, their ordinate, or both. Abscissa labelling is the factory default setting. Ordinate labels include the units; abscissa labels do not.

How the labels are located

The positions of peak labels are determined by the following rules:

1 For automatically-selected peaks, maxima are labelled above the peak and minima below.

2 For manually-selected positions, absorbance spectra and interferograms are labelled above the peak, and %T and single-beam spectra below.

3 The label is located where it will not overwrite the axis or go outside the plot window. This rule overrides the first two. However, if the label can only be located so that it overwrites the axis or goes outside the plot window, the position is determined by rules 1 and 2 above. (You may be able to overcome this problem by moving the spectrum up or down on the screen.)

Choosing the Peaks Option settings

1 At Ready For Next Command, press *setup* *plot* *OTHERS* *peaks*.
The command line and soft keys in Figure 4-17 appear.

Figure 4-17 Command Line and Soft Keys for the Plot Peaks Option

2 If you do not want to use the current **labelling** and **peak pick**, choose one of the other settings.

3 Press *EXECUTE* *EXIT*.
Ready For Next Command returns.

Plotting Spectra using Different Line Colors

If you are using a color plotter, you can use different colors to plot not only the different spectra in a plot, but also the components of the text, for example, the axes and caption.

When a plot contains more than one spectrum, the comment for each spectrum is written with the pen that corresponds to that spectrum.

Color selection for plotting is by pen number:

1	2	3	4	5	6	7	8
Black	Red	Green	Blue	Yellow	Magenta	Cyan	Black

The black used in color graphics is composite black (yellow + magenta + cyan) rather than from the black cartridge, and is not as intense as true black.

You can switch off the logo by setting its color to **0**; otherwise, you cannot control its color.

1 At Ready For Next Command, press ***setup*** (*plot*) (*OTHERS*) (*pens*) .
The command line and soft keys in Figure 4-18 appear.

Figure 4-18 Command Line and Soft Keys for the Plot Pens Option

2 Press ***enter*** repeatedly until the alphanumeric cursor is in the first field whose pen selection you want to change.
The cursor moves one field to the right each time that you press ***enter*** .

3 Type a number from 1 to 8, corresponding to a pen position in your plotter.

4 Press ***enter*** to move the cursor to the next field you want to change.

5 Repeat steps 3 and 4 until the command line is correct.

NOTE: *You can set a color for the grid that the spectra are plotted over if you have* **plot grid** *switched on. The best results for the grid are with* **plot pens grid** *set to* **5**, **6**, *or* **7** *(yellow, magenta, or cyan). the best results for the spectra are with* **plot pens spectra** *set to* **2**, **3**, *or* **4** *(red, green, or blue).*

6 Press (*EXECUTE*) (*EXIT*) .
Ready For Next Command returns.

Quality

You can choose to plot a *draft* quality spectrum: the spectrum is plotted more quickly because only half of the data points are used.

1 At Ready For Next Command, press **setup** (plot) (OTHERS) (quality) .
The command line and soft keys in Figure 4-19 appear.

Figure 4-19 The Plot Quality Command Line and Soft Keys

2 If you do not want to use the current setting, choose the other setting.

3 Press (EXECUTE) (EXIT) .
Ready For Next Command returns.

NOTE: *For color deskjet printers, choosing draft quality will give a monochrome plot. This can be up to 3 times faster than a color plot.*

Rotating a Plot

You can choose the orientation of the plot:

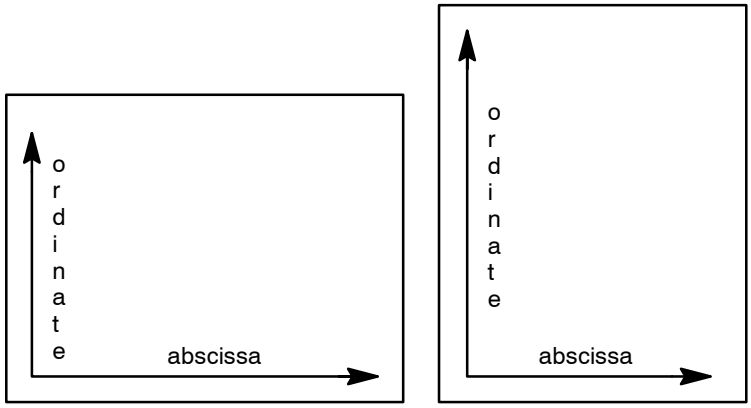

Figure 4-20 Orientation of Plots on $8^{1}/_{2}$ x 11 inch Paper

1 At Ready For Next Command, press **setup** (plot) (rotate).
The command line and soft keys in Figure 4-21 appear.

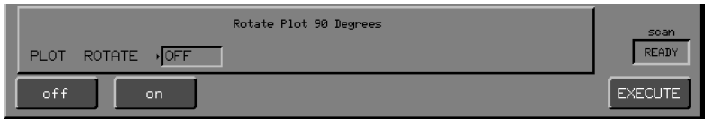

Figure 4-21 The Plot Rotate Command Line and Soft Keys

2 If you do not want to use the current setting, choose the other setting.

NOTE: *If you change the setting, you must then reset the Plot Window option. If the window is set to* **single***, for example, display the Plot Window command and press* **single** *again. The dimensions of the window are then reset so that they are appropriate for the rotated plot.*

3 Press (EXECUTE) (EXIT).
Ready For Next Command returns.

NOTE: *The caption is rotated automatically. If you do not want it to be rotated, press* (caption) (reset).

Setting the Position of a Plot using Plot Window

You can set the position of the plotted axes on the paper either by using one of the pre-set positions, or by setting the distance of the axes from the bottom left-hand corner of the paper.

Pre-set positions

The six pre-set positions (Table 4-2) correspond to the six plot windows that you will probably use most often, so you do not have to calculate their dimensions. However, if you change the orientation of the plot (using Plot Rotate) you must set the Plot Window again.

Soft Key	Position of Plot
single	The plot covers the largest possible area. (This is the factory default.)
top	The available area is divided in half, and the plot is
bottom	in either the top or the bottom half.
high	The available area is divided into thirds, and the plot is
mid	in the top, middle or bottom third.
low	

Table 4-2 Plot Window Soft Keys

User-defined positions

The end points of the axes are defined by specifying their distance, in mm, from the bottom left-hand corner of the paper. Figure 4-22 shows the four Plot Window parameters (two for each axis):

xleft distance from the left-hand edge of the paper to the left-hand end of the abscissa axis.

xright distance from the left-hand edge of the paper to the right-hand end of the abscissa axis.

ylo distance from the bottom edge of the paper to the bottom of the ordinate axis.

yhi distance from the bottom edge of the paper to the top of the ordinate axis.

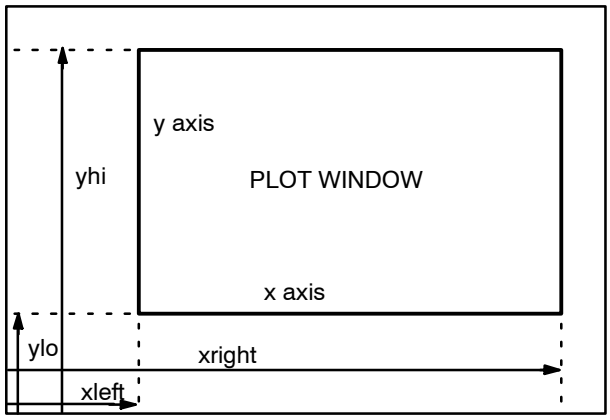

Figure 4-22 Setting the Positions of the Axes

Specifying a location for the plot window

1 At Ready For Next Command, press **setup** **plot** **window** .
The command line and soft keys shown in Figure 4-23 appear.

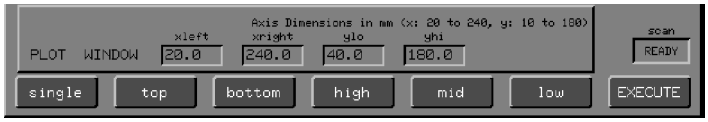

Figure 4-23 The Plot Window command line and soft keys

2 Choose one of the six pre-set plot windows (Table 4-2).
The first Plot options screen returns.

Specifying a custom plot window

3 Type the distance of the left-hand end of the abscissa axis from the left-hand edge of the paper (**xleft**) (Figure 4-22).

4 Press **enter** .

5 Repeat for **xright**, **ylo**, and **yhi**, using Figure 4-22 to help determine the correct setting for each.

6 When all fields are as you need them, press **EXECUTE** **EXIT** .
Ready For Next Command returns. If your window exceeds the window dimensions suggested in the title of Plot Window, a warning appears: **standard paper size exceeded**.

If you are using a LaserJet or a Desk Jet printer

If you are plotting two or three spectra on a page, the Plot Window option must be set differently for LaserJet and Desk Jet printers. It is particularly important to remember this if you have created a method that includes plotting to one of these types of printer, because the printout will be different if you connect the other type of printer.

For a LaserJet, choose one of the pre-set Plot Window options in the usual way

For a Desk Jet, note that when it has completed a plot, the printer treats its current position as the top of the page. For example, if you are plotting three spectra on a page, the first spectrum is plotted at the top of the page (**high**), and the Desk Jet is then ready to plot in the **mid** window. But, because it treats its current position as the top of the page, the Plot Window option must be set to **high** again, otherwise the spectrum will be plotted in the **low** window.

NOTE: *Make sure that you also position the caption correctly for the Desk Jet.*

Plotting

1 If necessary, use the Plot options in Setup to change the plot parameters (see *Setting up the Plotter*, starting on page 4-5).

2 Adjust the screen display until it represents the spectrum region(s), the abscissa range, and the ordinate scale you want to plot.

3 If your plotter has a rack for pens of different colors, position the pens as you want them.

4 Press **plot**.
If you use the factory-set plot parameters, the plot is similar to Figure 4-24.

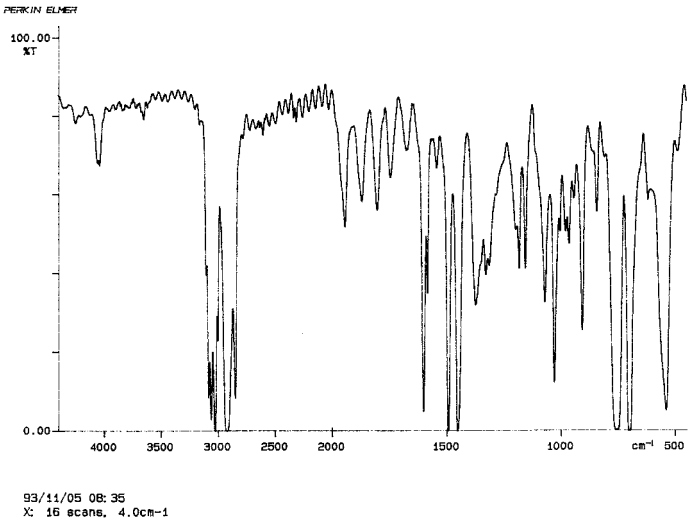

Figure 4-24 Typical Plot, Using the Factory-set Plot Parameters

Stopping the plot

1 Press **cancel**.
Soft keys appear corresponding to all the detached tasks that are running.

2 Press **plot**.
Or, if you decide not to cancel, press **EXIT**.

Introduction to Printing

There are three ways that you can print using the Spectrum RXI:

- by pressing print ; using the Print setup options you can choose whether text, graphics, or the entire contents of the screen are displayed.
- by automatically printing the scroll buffer as it is created; you can print commands, results, or errors, or all three.
- by pressing print when, for example, you are generating a peak table or the results of a Quant analysis. When you press print , the peak table or Quant results are generated and printed.

The output is sent to the device designated as **printer** in the Device options of Setup; this device can be a printer, a plotter, or an external computer. Before you can use a printer connected to the Spectrum RXI, you must configure the Spectrum RXI for that printer (see *Configuring the Spectrum RXI for Peripheral Devices* in *Advanced Operations*).

NOTE: *The following devices support HPGL, and can therefore be used as a printer or a plotter: HP LaserJet III, HP LaserJet IV and Paintjet 1200.*

Setting up the Print Options

The Print options specify what is printed when you press print, and enable you to set up automatic printing of various types of output.

Setting the Type of Output that is Printed

Three types of output can be printed:

text print sends the displayed portion of the scroll buffer to the device configured as **printer** in the Device options.

graph print sends the graphics display to the device configured as **printer** in the Device options.

screen print sends the entire contents of the screen to the device configured as **printer** in the Device options.

You can also choose whether you want the printer to do a *form-feed* (feed in the next sheet of continuous-feed paper) after each print.

NOTE: *If the screen is being printed on a LaserJet or DeskJet printer, you can customize the quality of the output. The two options are:*

- *the default, which prints more quickly and provides a good representation of the screen;*
- *higher quality output, which uses a gray scale, or dithered color dots, to provide a* true color *representation of the screen. To set up this option, press* setup OTHERS devices printer centron custom format*, and set* **type** *to PCL or PCL5. If* **type** *is PCL, set dpi to 300; if* **type** *is PCL5, dpi is automatically set to 300.*

Choosing the type of output

1 Press *setup* *OTHERS* *print* *key* .
The command line and soft keys in Figure 4-25 are displayed.

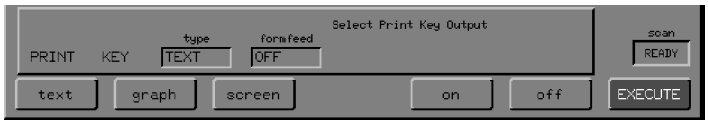

Figure 4-25 The Print Key Command Line and Soft Keys

2 If you do not want to use the current settings, choose other settings.

3 Press *EXECUTE* *EXIT* .
Ready For Next Command returns.

Automatically Printing Output

You can use automatic printing to create a daily log of your commands and their results, to help with debugging during development of a new method file, or to determine the situations that are causing error messages to appear.

The Print Auto option sets up automatic printing of any or all of the following types of output as they enter the scroll buffer:

commands – An echo of each command executed is printed.

results – Each result that is generated is printed.

errors – Each error message is printed.

NOTE: *Make sure that the printer is connected and switched on whenever you switch on automatic printing. If the printer is not ready, the Spectrum RXI pauses after each attempt to print, and it works very slowly.*

NOTE: *When output is printed automatically, the printer only does a form-feed when the current sheet of paper is full.*

Setting up automatic printing

1 Press *setup* *OTHERS* *print* *auto* .
The command line and soft keys in Figure 4-26 are displayed.

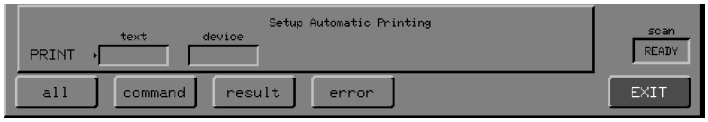

Figure 4-26 The Print Auto Command Line and Soft Keys

2 If you want commands, results, and errors all to print automatically, press *all* .
Otherwise, choose the one type of output you want to print.
The cursor moves to the **device** *field. The command line and soft keys in Figure 4-27 are displayed.*

Figure 4-27 The Print Auto Devices Command Line and Soft Keys

3 Choose the device to be used for output, or press *off* to switch off automatic printing.
The table is updated, then the Print Auto screen returns.

4 Press *EXIT* *EXIT* .
Ready For Next Command returns.

Printing using print

1 If necessary, use the Print options in Setup to change the print parameters (see *Setting up the Printer*, starting on page 4-29).

2 If you have configured a plotter to receive the output of Print, make sure that the pen is down and in position at the left-hand side of the paper.

3 Press print.
The device designated as **printer** *in Setup Devices prints the part of the screen specified by the Print Key option of Setup. If the* **formfeed** *option is switched on, the paper then advances to the next sheet.*

Copying and Storing Data 5

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Introduction

This chapter describes how to copy and store data, and how to format a disk.

More advanced disk operations, such as listing the files in a directory, searching for a file, creating a new directory, changing the working directory, backing up, formatting and labelling disks, and renaming a file or directory are described in *Using the Disk Drive*, in *Advanced Operations*.

Copying Files

The Copy command transfers either spectral data or method files from one location to another. The data remain in the original location, and the Spectrum RXI places a copy in the destination.

NOTE: *When you are copying files, you may want to view the contents of the file before you copy them. To do this, press* preview *, then press* ENTER *to select that file, or* reselect *to return to the screen for selecting a file.*

1 At Ready For Next Command, press copy.
The command line and soft keys in Figure 5-1 are displayed, with the cursor at the **from** *field.*

Figure 5-1 The Command Line and Soft Keys for Copying Files

2 Choose the source of the file to be copied:

- To choose a spectrum region, press one of the region keys.
- To choose a store region:

  a Press store.
  A list of the store regions and their contents, and the soft keys for choosing a store region, are displayed.

  b Press one of the store region keys.
  The contents of the store region are displayed.

  c Press ENTER.

- To choose a disk or the notepad, press (disk) then choose the file to copy (see *Copying a File from a Disk* on page 5-4).

The cursor moves to the **to** *field, and the soft keys for choosing a destination are displayed.*

If you are copying a method file, the method region keys are displayed, and you can copy the method to an empty region or overwrite a current method.

NOTE: *Before attempting to copy to or from a device connected to the RS232 port, for example, a computer or modem, make sure that the port is configured. To do this, use the Device Options of Setup as described in Chapter 2 of* Advanced Operations.

3 Choose a destination for the file:

- To choose a spectrum region, press one of the region keys.
- To choose a store region:

  a Press (store).
  A list of the store regions and their contents, and the soft keys for choosing a store region, are displayed.

  b Press one of the store region keys.
  The contents of the store region are displayed.

  c Press (EXECUTE).
- To choose a disk or the notepad, press (disk) then choose the file to copy (see *Copying a File to Disk* on page 5-6).

The file is copied, and Ready For Next Command returns.

Copying a File *from* a Disk

1 Press **copy** (disk) .
The screen for choosing a file from a disk is displayed. The filename of the first file in the working directory is in the **from** *field.*

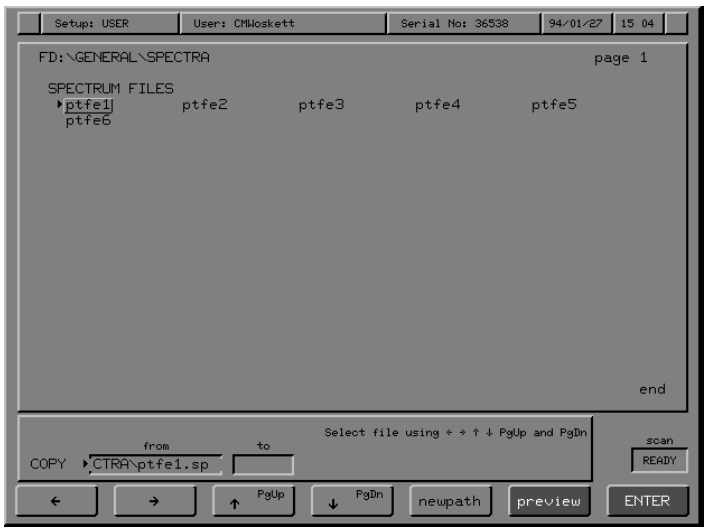

Figure 5-2 Screen for Choosing a File from a Disk

2 Choose the file that you are going to copy:
- To choose the current file, press ENTER .
- To choose another file from the working directory:

  a Use the arrow keys to move the highlight through the file list.
  When a name is highlighted, it is also displayed in the **from** *field.*

  b Press ENTER .
- To choose a file from a different directory, press (newpath) to display the directory tree (see *To change directory,* on the next page).

3 Press ENTER .

To change directory

If you want to choose a file that is in a different directory or the notepad, change directory as follows:

1 Press (newpath) .
A directory tree is displayed, showing the working directory, which is indicated by the cursor.

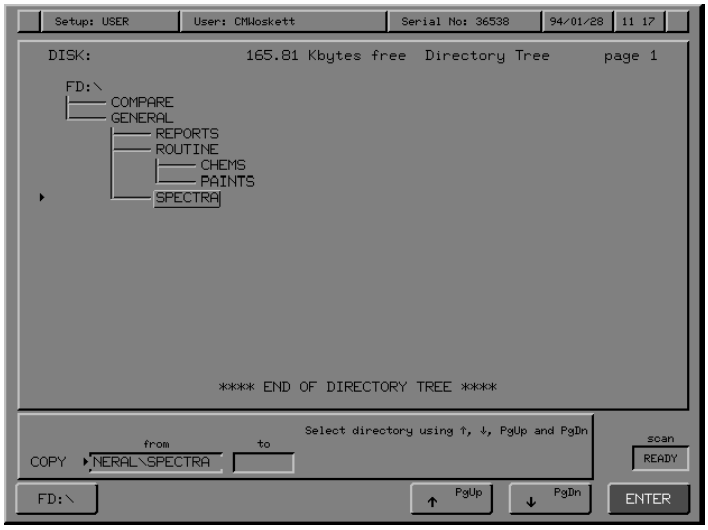

Figure 5-3 Screen for Changing Directory

2 Use (pgup) and (pgdn) to highlight a directory.
When you move the cursor away from the working directory, (reset) is displayed; press it to return the cursor to the working directory.

3 Press (ENTER) .
The list of files in the directory is displayed. If the directory is empty, press (newpath) to display the directory tree again.

4 Use the arrow keys to move the highlight through the list of files.
When a name is highlighted, it is also displayed in the **from** *field.*

5 Press (ENTER) .
The Copy screen returns.

Copying a File *to* a Disk

1 With the Copy screen displayed (and the required filename in the **from** field), press (disk) .
The files in the working directory are listed.

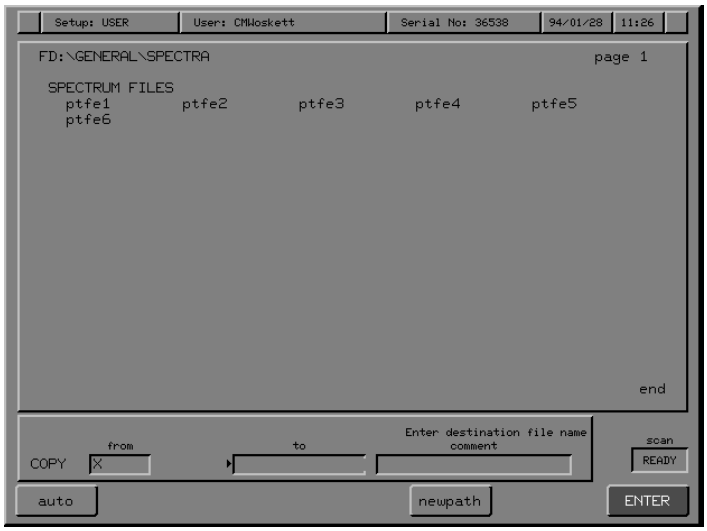

Figure 5-4 List of Files in the Working Directory

2 To overwrite a file, enter the filename in the **to** field.

or

Delete the current filename and type a new filename.

or

Use (auto) (see the next page) to generate filenames automatically.

or

Press (newpath) to change directory, as described for *Copying a File from a Disk* on page 5-5.

3 Press ENTER .
The cursor moves to the **comment** *field,* auto *and* newpath *disappear, and* recall *appears.*

If you will overwrite a file, the following message is displayed:
Error: duplicate filename: press CONTINUE to overwrite.
Alternatively, press CANCEL *to cancel the copy.*

4 Type a comment, or press recall to display the comment previously stored with that file.

5 Press EXECUTE .
The file is copied and Ready For Next Command returns.

Generating filenames automatically

You can use auto to save spectra or interferograms to sequentially-named files in the current working directory. To use auto :

1 Type a family filename, for example **PAINT-**.

NOTE: *The family filename can have up to five characters if you want to have up to 999 files in the "family", for example, if it is* **POLY-**, *the automatic filenames will be* **POLY-001, POLY-002** *and so on; the family filename can have up to six characters if you want to have up to 99 files in the "family", for example, if it is* **PAINT-**, *the automatic filenames will be* **PAINT-01, PAINT-02** *and so on.*

2 Press auto ENTER .
The cursor moves to the **comment** *field,* auto *and* newpath *disappear, and* recall *appears.*

3 Type a comment.

4 Press EXECUTE .
The file is copied and Ready For Next Command returns.

When you want to copy the next file from, for example, spectrum region X to that directory:

* Press copy X disk auto .
The filename in the **to** *field automatically increases.*

Formatting a Disk

Disks formatted on the Spectrum RXI are compatible with IBM PCs. To format a blank disk or reformat a used one, set the disk options, if necessary, then:

1 Insert the disk to be formatted into the disk drive.

2 At Ready For Next Command, press **setup** (OTHERS) (disk) (format) .
The command line and soft keys in Figure 5-5 are displayed.

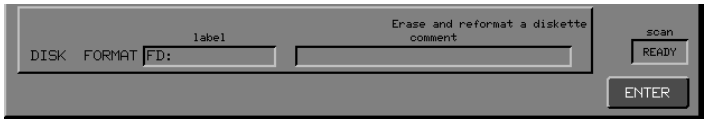

Figure 5-5 The Command Line and Soft Keys for Formatting a Disk

3 If you want the disk to have a volume label, type the name in the **label** field.

NOTE: *The volume label must not contain any spaces.*

4 Press (ENTER) .
The cursor moves to the **comment** *field*

5 If you want to include a comment about the disk, type the information in the **comment** field.

6 Press (EXECUTE) .
A progress bar and a (detach) key appear.

* If you want to use the Spectrum RXI for other tasks while the disk is being formatted, press (detach) .
The Disk Options Screen returns. When the format is complete, the beeper sounds and the following message is displayed: **disk format complete**.

* To cancel a detached formatting task, press **cancel** twice.
Action keys appear corresponding to the detached tasks in progress.

When formatting is complete, (detach) disappears and the Disk Options return.

Methods 6

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Introduction

A method comprises a list of commands; when you select the method, the commands are automatically executed in sequence by the Spectrum RXI. For example, methods can be used to:

- simplify complicated analyses by issuing the user with prompts and information during an analysis.
- make sure that repetitive analyses are always performed using the same conditions, and generate a report of an analysis.

You are provided with some example methods, which are described on page 6-13.

The Spectrum RXI contains 27 KB of memory for methods. The memory is divided between the seven method regions in the proportions required by the individual methods. If the 27 KB of memory is filled by only, for example, five methods, then you can only store those five methods. In this situation, you cannot copy another method into a method region, even if there is an empty one; you must erase one or more of the current methods to create free memory.

Methods are not lost when you switch off the Spectrum RXI; when you store a method in a method region, it remains available for use until you erase it.

In this chapter

This chapter tells you how to:

- run methods
- rename methods
- copy methods to and from the method regions
- erase methods from the method regions
- print methods
- lock the Spectrum RXI so that only the methods are available.

Using Methods

The Spectrum RXI has seven method regions. You can run any of the methods in these seven method regions as follows:

1 Press ***method*** .
Soft keys are displayed that represent the methods stored in the Spectrum RXI.

Figure 6-1 Action Keys for Starting Methods

2 Press the action key corresponding to the method you want to use.
The Spectrum RXI begins executing the method. As each command executes, it is listed in the Previous Command Line. When the method has finished, Ready For Next Command returns.

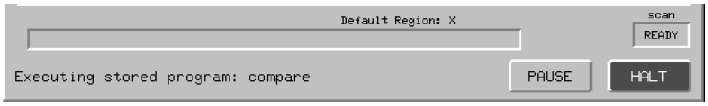

Figure 6-2 Command Line and Soft Keys when a Method is Running

NOTE: *If the method you want to run is stored on disk and is not currently in a method region of the Spectrum RXI, use* ***copy*** *to place it in a method region (see Copying Methods on page 6-5).*

Stopping a Method

Temporarily

To stop a method temporarily:

1 Press (pause) .
The method pauses, and (proceed) is displayed.

2 Press (proceed) when you are ready to resume the method.

Permanently

To stop a method permanently:

* Press (STOP) .
The method stops. Any data or results already generated by the method are kept.

Erasing Methods

If you no longer need a method, you can erase it. If you want to save the method for future use, store it on disk before you erase it (see *Copying Methods* on page 6-5). If you have no disk drive, print a hard copy of your files (see *Printing Methods* on page 6-11).

1 Press **setup** **method** **erase** .
The Method Erase screen is displayed, with soft keys that contain the names of current methods. (No keys appear for method regions that are empty.) The current methods and the size of each are listed, so that you know how much memory you will gain by erasing each one.

2 Choose the method you want to erase.
The method is listed, and an **EXECUTE** *key appears (Figure 6-3).*

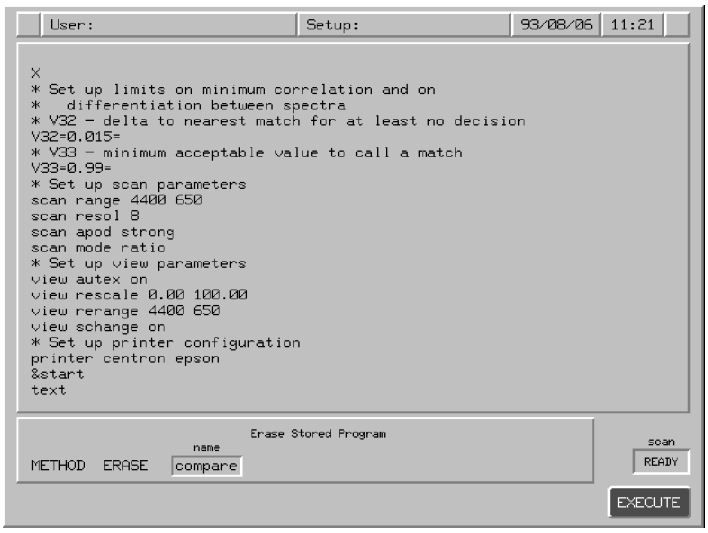

Figure 6-3 Erasing a Method

3 Press **EXECUTE** .
The method is erased from the method region. The Method Options screen returns.

Copying Methods

You can store up to seven methods in the method regions of the Spectrum RXI. If you have more than seven methods, you must store some of them on a disk or computer, and copy them to the method regions when you need them.

There are three commands that you can use to copy methods to the method regions: the **copy** hard key, the Method Copy command, and using instrument configuration files. The **copy** hard key is quicker to use because you press fewer keys, but it can only be used to copy methods from disk. If you want to copy methods from a computer you must use the Method Copy command.

Instrument configuration files (see page1-14 of *Advanced Operations*) enable you to save all of the settings of your Spectrum RXI, including the methods stored in the method regions, to a file.

Copying a method from disk

1 Press **copy**.
The Copy command line and soft keys appear (Figure 6-4).

Figure 6-4 The Copy Command Line and Soft Keys

2 Press **disk**.
A list of the files in the current disk directory appears and the filepath of the first file appears in the **from** *field (Figure 6-5).*

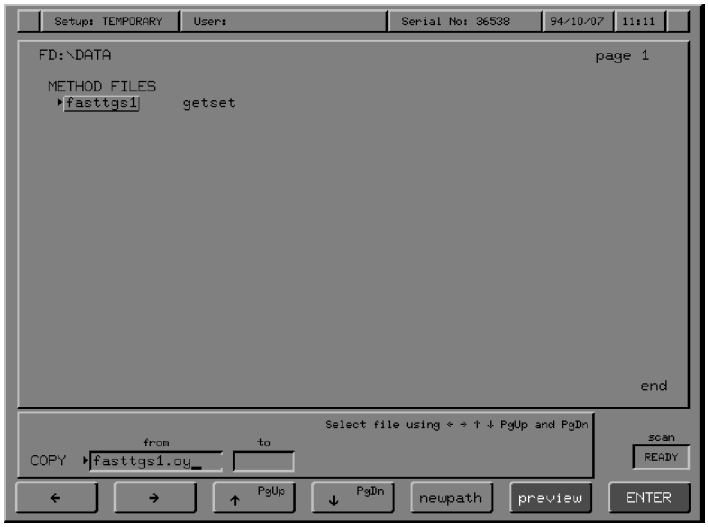

Figure 6-5 The List of Files in the Current Directory

3 If the method you want to copy is in a different directory or on a different disk:

a Press ***newpath*** .
A list of the directories on the current disk appears.

b Use the arrow soft keys to select the directory that contains the method.

c Press ***EXECUTE*** .
The list of files in the directory you selected appears.

4 Use the arrow soft keys to select the method that you want to copy.

5 Press ***ENTER*** .
The contents of the Method you selected appear. Action keys, corresponding to the empty method regions, and soft keys, corresponding to the method regions containing methods, appear (Figure 6-6).

Figure 6-6 Choosing the Destination of the Method

6 Press an action key that corresponds to an unused method region.

or

If you want to overwrite one of the methods, press the soft key that corresponds to that method, and press EXECUTE.
The method is copied from disk into the method region that you chose.

Copying a method from a computer

1 Press setup method copy.
The Method Copy screen appears (Figure 6-7). The current methods and the size of each are listed, and the total number of bytes remaining is reported. The soft key cursor indicates that you are about to enter the source of the method in the **from** *field.*

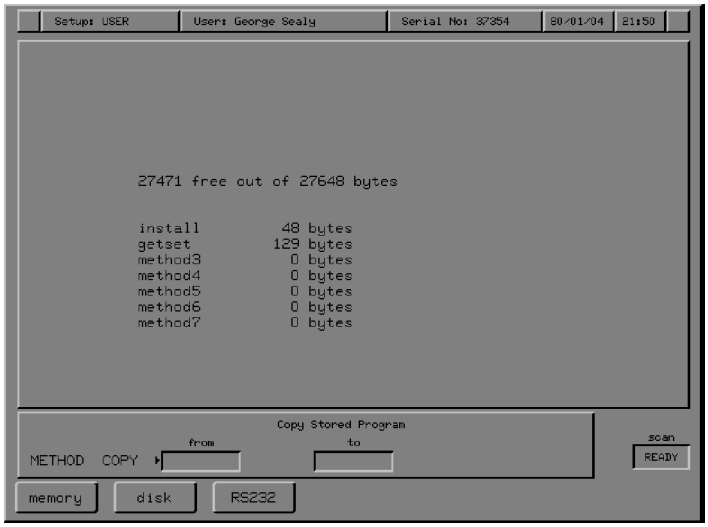

Figure 6-7 The Method Copy Screen

2 Make sure that the RS232 port is configured, and that the timeout is set to at least 10 seconds (see *Communicating with Other Devices*, in *Advanced Operations*).

3 At the DOS prompt on the computer, type **copy <filename> com1:** (Do not press ***Enter*** on the computer keyboard yet.)

4 On the Spectrum RXI keypad, press ***RS232*** .
Action keys, corresponding to the empty method regions, and soft keys, corresponding to the method regions containing methods, appear.

5 Press an action key that corresponds to an unused method region.

or

If you want to overwrite one of the methods, press the soft key that corresponds to that method, and press ***EXECUTE*** .

6 Press ***Enter*** on the computer keyboard.
The method is copied, and the Method Options screen returns.

Additional Information About Copying

Names for methods

When you copy a method file into a method region, the following rules are used to name the method.

- If the source was either RS232 or another method region, the copy is given a default name (for example, **method3**) .
- If the source was a disk file, the filename is assigned to the method region. If that name is already in use, the copy receives a default name, for example, **method2**.

Choosing a file from the disk

The screen for choosing a file from a disk is shown in Figure 6-8.

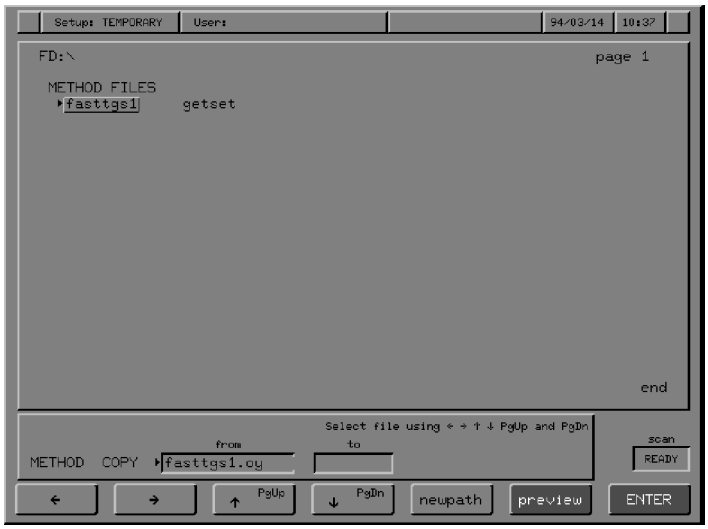

Figure 6-8 Screen For Selecting A File From a Disk

- The arrow keys move the highlighting through the menu of filenames. As each name is highlighted, it is also displayed in the **from** field.
- If there are more filenames on the disk than fit on one screen, press ***shift*** (***pgup***) .
- If you decide that the file is on a different disk, put the new disk in the drive, and press (***newpath***) .

Renaming Methods

You can rename a method in a method region as follows:

1 Press **setup** **method** **rename** .
Soft keys are displayed corresponding to the names of existing methods. (No keys are displayed for method regions that are empty.)

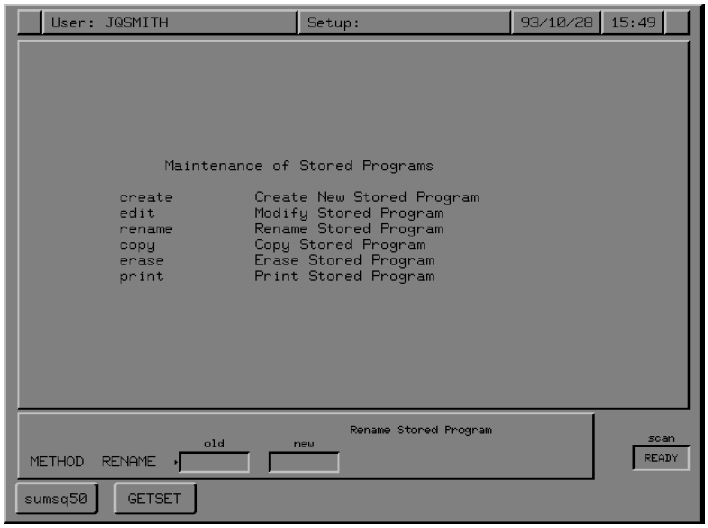

Figure 6-9 The Method Rename Screen

2 Press the soft key that represents the method you want to rename.
The name is displayed in the **old** *field. The cursor moves to the* **new** *field.*

3 Type the new name for the method. When it is complete, press **enter** .
The command executes, and the Method Options screen returns.

Printing Methods

1 Make sure that the printer is switched on, and that the paper feed is set to the beginning of a sheet.

2 Press ***setup*** (***method***) (***print***).
Action keys are displayed corresponding to the names of existing methods. (No keys appear for method regions that are empty.) The current methods and the size of each are listed,

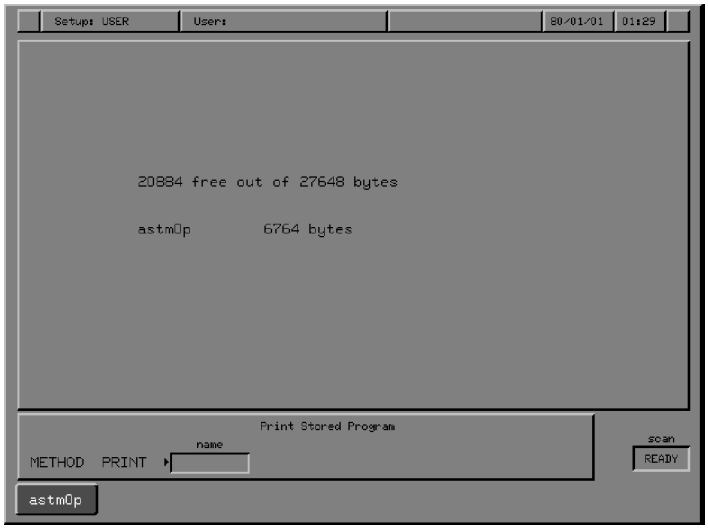

Figure 6-10 The Method Print Screen

3 Press the soft key corresponding to the method you want to print.
A copy of the method is printed. The header includes the name of the method, the date and time, and a page number. The printed method includes line numbers, for convenience in editing.

Locking the Keypad for Methods

You can lock the keypad of your Spectrum RXI so that it can only be used to run methods.

Setting up the lock

1 At Ready For Next Command press
setup (OTHERS) (OTHERS) (misc) (locks).
The command line and soft keys in Figure 6-11 are displayed.

Figure 6-11 The Lock Options Command Line and Soft Keys

2 Press (method).
Action keys for the stored methods are displayed.

3 Press (EXECUTE) (EXIT).
Ready For Next Command returns, with the action keys for the stored methods still displayed.

Removing the lock

1 To remove the lock, press **restore** (keypad).
Ready For Next Command returns.

Example Methods

A disk of example methods was supplied with your Spectrum RXI. It contains methods that you may find useful.

Descriptions of Example Methods

Quantitative analysis

The method quant.oy is a turnkey method for Beer's Law quantitative analysis; the method and seven example standard spectra are stored in the subdirectory FD:\BEERSLAW.

quant.oy performs quantitative analyses of defined spectrum peaks, based on Beer's Law. This states that the absorbance measured by the spectrometer (A) is proportional to the absorptivity of the analyte (α), the pathlength of the cell or thickness of the sample (b) and the concentration of the analyte (c):

$$A \propto \alpha\, b\, c$$

The method determines a calibration curve relating the absorbance measured and the concentration of the sample, by linear regression, from spectra of samples of known calibration and pathlength. The method then uses the slope and intercept of the calibration curve to calculate the concentration of samples.

Beer's Law Quantitative Analysis can be applied to analytes where well-defined peaks can be located by the analyst.

The method also enables you to choose the scan parameters when collecting spectra, choose the type of analysis performed on the peaks (peak height, peak area, ratioed peak height and ratioed peak area), store your standard spectra on disk, and produce calibration and analysis reports.

The features of this method are:

- Control of scanning parameters such as number of scans and resolution to make sure that data are collected repeatably;
- Four modes of analysis (peak height, peak area, ratioed peak height and ratioed peak area) for a variety of sample types;
- Definition of peak and baseline frequencies;
- Storage and retrieval of standard spectra from disk, with a recalculation option which enables standards to be added, removed or changed from the stored calibration information;
- The complete Method Report documents the analysis mode, peak and baseline frequencies used, and data collection parameters;
- Variable number of standards from two to twenty;
- Calibration Report prints absorbance and concentration of each standard used, the slope, intercept and correlation coefficient from the linear regression calculation and a plot of the calibration curve;
- Analysis Report with a date/time stamp, the measured absorbance and computed concentration and a plot of the acquired spectrum;

The special requirements for this method are:

- The Spectrum RXI must have a printer, and be capable of running methods.
- The program as distributed requires approximately 14 KB of method memory.

For more information about this method, contact your Perkin-Elmer office or agent and ask for Application Note FT 19.07.

Materials verification

Two turnkey methods for materials verification are provided: compare.oy and setmeth.oy. The methods, example standards, and control spectra are stored in the subdirectory FD:\COMPARE.

setmeth.oy sets up the Spectrum RXI to run the compare.oy method. Once you have run it, it does not have to remain in memory while you run compare.oy.

compare.oy uses a patented algorithm to discriminate between two closely-related spectra, to determine if they are from the same material. It minimizes the features of the spectrum caused by the method of collection, and maximizes the differences caused by contaminants or adulterants in the materials.

The features of these two methods are:

- Patented algorithm for discriminating real differences between infrared spectra;
- Complete control of data collection and method parameters, including scan range, resolution, spectral comparison range;
- Collection of control, accessory and background reference spectra limited to supervisory program;
- Instrument, control and accessory checks to ensure system suitability;
- Pass/Fail/No Decision reports for material verification;
- COMPARE a sample and reference spectrum or a sample and all reference spectra stored in a directory;
- User-defined correlation and discrimination factors allow broad or narrow classifications of materials.

The special requirements for these methods are:

- The Spectrum RXI must have a printer, be capable of running methods, and have the Compare software installed.
- The programs as distributed require approximately 18 KB of method memory. The setmeth program requires approximately 8 KB, but need not be in method memory when the Compare method is executed, so approximately 10 KB are required at run time.

For more information about these methods, contact your Perkin-Elmer office or agent and ask for Application Note FT 19.02.

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