Spectra Analysis Program

Instruction Manual

JASCO Spectrometers for Windows®

JASCO

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Contents

1 Introduction

1.1 About This Manual

This instruction manual is intended to serve as a guide for operating the JASCO Spectra Analysis program and the JASCO File Find program, both designed to run on Microsoft Window 95/98/NT4.0. This manual consists of three sections (including this section) and an appendix. The contents of each section are briefly described below.

The JASCO Spectra Analysis program can be used with various JASCO spectrometers, for example, UV/VIS and UV/VIS/NIR spectrophotometers, spectrofluorometers, FT/IR and Circular Dichroism spectropolarimeters. The screen examples used throughout this manual are taken from screens displayed when the JASCO Spectra Analysis program is used with a UV-Visible spectrophotometer. That is, either absorbance or transmittance are shown on the abscissa (vertical axis). When using the JASCO Spectra Analysis program with a different spectrometer, the relevant abscissa will be displayed. For example, for a spectrofluorometer intensity will typically be displayed on the abscissa.

Note: Refer to the Measurement manual for notation conventions and how to open and close the program.
The Measurement manual describes procedures ranging from measurement to spectrum analysis. Refer to it, as and if necessary.

1 Introduction
Contains a description of how to use this manual, an overview of the Spectra Analysis program, and the screen configuration and basic operation of the Spectra Analysis program. Read this section first.

2 Spectra Analysis Program: Reference
Contains reference information for the Spectra Analysis program. The Spectra Analysis program performs data processing operations such as peak find, difference spectrum calculation, differentiation, and smoothing.

3 File Find Program: Reference
Contains reference information for the File Find program. The File Find program is used to search for a previously saved spectrum.

4 Appendix
Contains various technical information for the Spectra Analysis program.

1.2 Spectra Analysis Program Overview

The main Spectra Analysis program functions are as follows.

(1) File functions: Save, load or print spectra.
(2) Edit functions: Copy a spectrum to the clipboard or between views. Delete a spectrum.
(3) View functions: Change spectrum characteristics such as the scale, color, or font. Display or hide peak find results.
(4) Data processing functions:

- Correction
  - Baseline correction: Corrects a spectrum with a designated baseline.
  - Smoothing: Smoothes the spectrum.
  - Noise elimination: Eliminates noise of known cause.
  - Deconvolution: Separates overlaid peaks.

FFT filter: Eliminates noise.
Data Cut: Cuts out unwanted data.

- Arithmetic
  - Arithmetic: Performs arithmetic operations between spectra or with a spectrum and a constant.
  - Derivative: Differentiates a spectrum.
  - KK conversion: Performs Kramers-Kronig conversion.

Note: The KK conversion function is only applicable for spectra for which the vertical axis is either absorbance(Abs), %T or %R.

- Peak
  - Peak find: Finds spectrum peaks (or valleys).
  - Peak height: Calculates the peak height and peak height ratio.
  - Peak area: Calculates the peak area and peak area ratio.
  - Peak width: Calculates the full width at half maximum value.
- Subtraction: Calculates a difference spectrum.
- X Unit Conversion: Converts the X-axis units of the spectrum.
- Y Unit Conversion: Converts the Y-axis units of the spectrum.

Note: The Y unit conversion function is only applicable for spectra for which the vertical axis is either or absorbance(Abs), %T or %R.

- Other
  - Comment: Adds/edits comments.
- Common options
  - Kinetics: Calculates enzyme activity.
  - Data Dump: Displays measured data values.
  - Move Channel: Move channels (for example, channel 1 and channel 2) in a view or pick up only data of a desired channel from data overlaid in a view or from multiple-channel data.
  - Arithmetic with Data: Performs arithmetic operation on data overlaid in the same channel of a View.
  - Arithmetic with Channel: Performs arithmetic operation on data displayed in the same View.
  - Data Accumulation: Accumulates the data overlaid in the same channel of a View and displays the accumulated data in a new View.
- IR Option
  - ATR conversion: Converts the absorption intensity relationship between the high wavenumber side and low wavenumber side.
  - IF -> spectrum: Converts an intrferogram(IF) into a single-beam spectrum.
  - Spectrum -> IF: Convert a single-beam spectrum into an interferogram(IF).
- FP Option
  - Phospho. Lifetime: Calculates the phosphorescent Lifetime.
- CD-options

HT → OD conversion	Converts HT voltage data into absorbance.
Optical constant calculate	Calculates optical constants.
KK conversion	Performs Kramers-Kronig conversion.
G Value	Calculates G value.
pH Conversion	Performs pH conversion.

1.3 [Spectra Analysis] Window

When the [Spectra Analysis] program starts up, the following window appears.

Note: Two or more windows may appear in order to display data. Each of these windows is referred to as a "View". Multiple data can be overlaid in one View.

Note: The [Spectra Analysis] program starts automatically when either spectrum measurement or time-course measurement is performed and the measurement data are displayed in a View window.

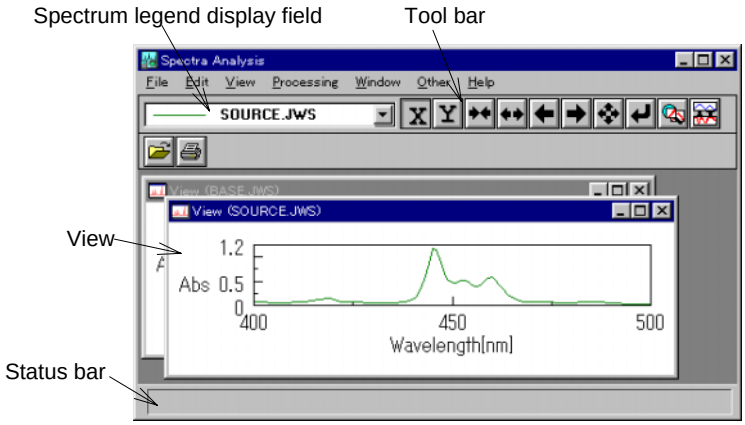


Fig. 1.1 [Spectra Analysis] window

Spectrum legend display	Displays the name of the active spectrum in the active View. Clicking the arrow at the right displays a list of all spectra overlaid in the View. Here, the active spectrum can be changed over.
Tool Bar	Contains buttons for frequently used functions. The buttons/functions described in Section 1.4 “Tool Bar” can only be found in the tool bar (i.e. they do not appear in the program menus). Other functions contained in the program menus can also be registered in the tool bar (up to a maximum of 10).
View	A window that displays a spectrum (or spectra). The filename of the active spectrum is displayed in the title bar of the View window.
Status bar	Displays the wavelength and data corresponding to the currently selected position. To select a position, move the mouse pointer to the desired position and click once with the left mouse button.

1.4 Tool Bar

The tool bar contains frequently used functions. In addition to the standard tool bar buttons, buttons corresponding to other functions contained in the program menus can also be registered (up to a maximum of 10). By clicking the appropriate button on the tool bar the corresponding function can be executed directly.
The first eight buttons below are used to change the scale settings.


Used to change x-axis scale.


Used to change y-axis scale


Reduces the spectrum horizontally (when  is depressed) or vertically (when  is depressed).


Expands the spectrum horizontally (when  is depressed) or vertically (when  is depressed).


Moves the spectrum to the left (when  is depressed) or up (when  is depressed).


Moves the spectrum to the right (when  is depressed) or down (when  is depressed).


Redisplays vertical axis at auto scale


Redisplays data at full scale (displays all regions).


Returns to default scale settings.


Activates the function for changing the scale using the mouse.


Changes the active data


Toggles between Overlay/Normalize
Normalize is used to display a spectrum with auto scaling.


Equivalent to [File]-[Open...]


Equivalent to [File]-[Print...]

Click the  button on the tool bar to change between active data.

Click the  button of the tool bar to switch between simple trace and spectrum extension functions.

The  button is not depressed during simple trace (i.e., the spectrum expansion function is off).
Press and hold the left mouse button at any position on the spectrum display. A vertical line appears at that position and the wavelength (or point) and data at that position are displayed in the status bar. The vertical line disappears when the mouse button is released. Use [Trace] in the [View] menu to trace all data points.

The  button is depressed during spectrum expansion (i.e., the spectrum expansion function is on)
Used the mouse to designate the expansion range. To designate the range, press and hold the mouse button at one of the corners of the desired range. Drag the cursor diagonally to the opposite corner. This creates a rectangular region which will

be expanded. Release the mouse button and the designated range is displayed. The scale changes accordingly. Click the right mouse button to return the display to its original scale. To designate a precise scale change, use [Scale] in the [View] menu.

2 Spectra Analysis Program Menu: Reference

To start the Spectra Analysis program, in the [Analysis] pane of [Spectra Manager] double-click on [Spectra Analysis]. The [Spectra Analysis] program starts up and the following window appears.

Note: The Spectra Analysis program can be used with various JASCO spectrometers, for example, UV/VIS and UV/VIS/NIR spectrophotometers, spectrofluorometers, FT/IR and Circular Dichroism spectropolarimeters. The screens and examples used in the descriptions throughout this manual are for spectra measured using a UV-Visible spectrophotometer (absorbance or transmittance on the abscissa). When using the Spectra Analysis program with a spectrofluorometer, emission intensity will typically be displayed on the abscissa.

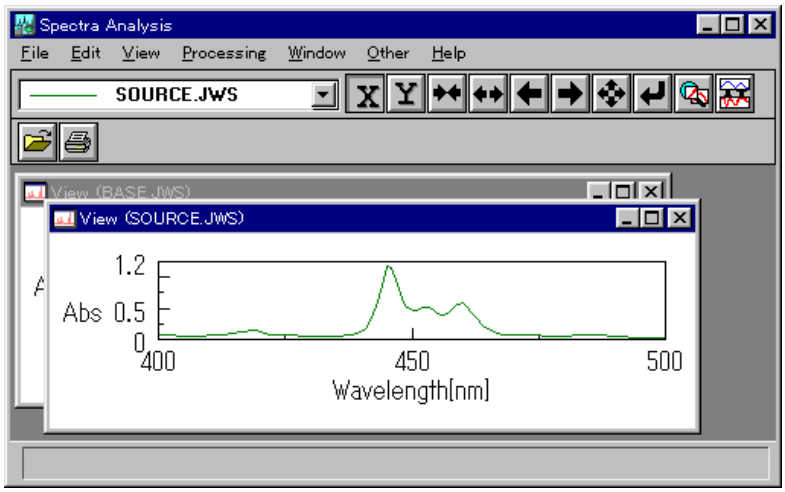


Fig. 2.1 [Spectra Analysis] window

2.1 [File] Menu

This section describes the commands contained in the [File] menu.

[Open...]	Displays the [Open New File] dialog box used to open previously saved spectra. Multiple files can be selected and opened at the same time.
[Overlay...]	Displays the [Overlay Additional File] dialog box used to add a spectrum to the active View. Multiple files can be selected and added at the same time.
[Close]	Closes the active View. If spectrum data have not been saved, a message prompt appears asking the operator whether to save the data before closing.
[Save]	Saves the active spectrum in the active View under the current filename. Previous data are overwritten.
[Save As...]	Displays the [Save As] dialog box used to save the active spectrum in the active View under a new filename and/or in a new location.
[Find...]	Starts the File Find program.
[Print...]	Prints the active spectrum.
[Print Preview...]	Displays the [Preview] dialog box which shows how the active view will look when printed.
[Print	Displays the [Print Setup] dialog box used to designate the

Setup...] target printer and set print parameters.

[Exit] Exits the Spectra Analysis program. If spectrum data have not been saved, a message prompt appears asking the operator whether to save the data before exiting.

2.1.1 [Open...]

Select [File] - [Open...] to display the [Open New File] dialog box used to open a spectrum (or spectra) in a new View. Multiple files can be selected at one time and opened in the same View or in separate Views.

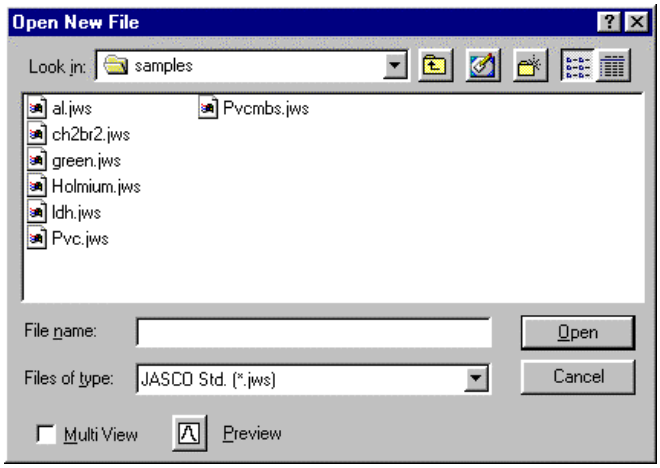


Fig. 2.2 [Open New File] dialog box

[Look in] Used to designate the drive or directory that holds the files you want. Available drives and directories appear in the drop-down list.
The contents of the drive or directory designated in the [Look in] drop-down list are shown in the box below. Select the desired spectrum file name. To select multiple non-sequential files, click on the desired spectra file names while holding down the [Ctrl] key. To select any number of sequential files click on the first and last file names of the desired list while holding down the [Shift] key. Spectra with different extensions cannot be selected simultaneously unless [All files] has been designated as the file type.

[File name] Used to directly input the desired spectrum filename(s). To select multiple files, input each filename separated by a space. The extension may be omitted. If an incorrect extension is input, the designated extension is substituted automatically.

[Files of type] Lists the file types (extensions) that can be opened with the Spectra Analysis program. If the extension is omitted when the file name is input, the file extension designated here is added automatically. When [All files] is selected, .jws is added automatically.

The following file types can be designated:

	Standard data (*.jws):	Data measured and calculated using the Spectra Analysis program.
	JCAMP-DX (*.dx):	Data in JCAMP-DX 4.24 format. Refer to JCAMP-DX Format Files for a description of the format that can be handled.
	All files (*.*):	Designates all files. Files not in one of the formats described above cannot be loaded.

[Multi View] Check to open multiple files in separate Views. If [Multi View] is not selected, the data are overlaid in a single View.

[Preview] Clicking the [Preview] button  displays a preview of the contents of the currently selected file and spectrum or information in file directory appears. When multiple files are selected, the preview pane displays the contents of the last file selected.

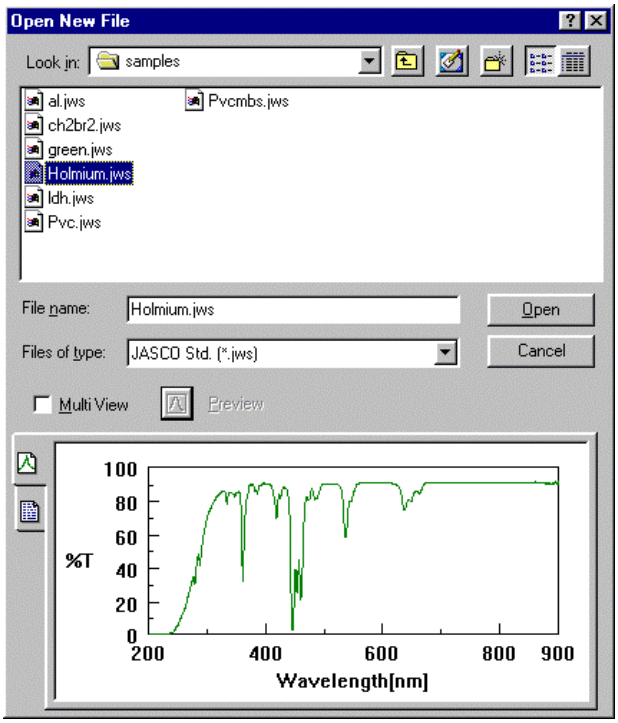


Fig. 2.3 [Open New File] dialog box showing the file preview pane

2.1.2 [Overlay...]

Select [File] - [Overlay...] to display the [Overlay Additional File] dialog box used to add a spectrum (or spectra) to the active View. Multiple files can be selected and added at the same time. The vertical axis is automatically re-scaled so that all of the spectra to be overlaid are displayed, however, the horizontal axis is not changed.

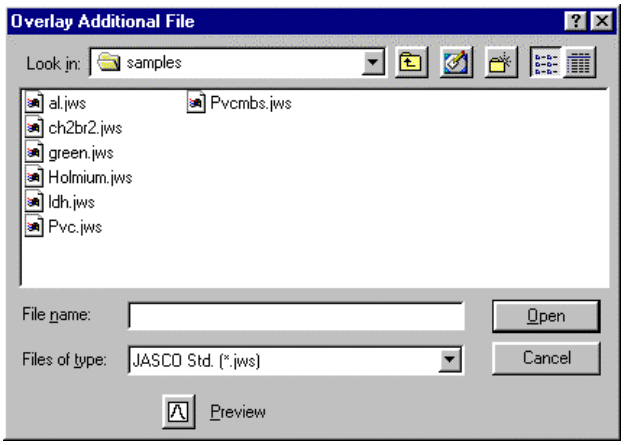


Fig. 2.4 [Overlay Additional File] dialog box

2.1.3 [Close]

Closes the active View. The following dialog box appears when there are spectra that have not been saved. Click [Yes] to save the spectra before closing. Click [No] to close without saving. Click [Cancel] to cancel closing the active View.

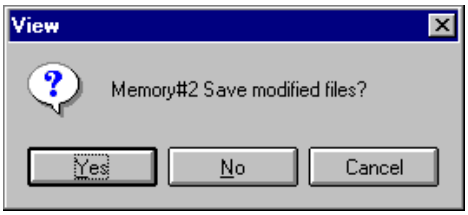


Fig 2.5 Message displayed before closing when there are spectra that have not been saved.

2.1.4 [Save]

Select [File] - [Save] to save the active spectrum in the active View under the current filename. Previous data are overwritten.

2.1.5 [Save As...]

Select [File] - [Save As...] to display the [Save As] dialog box used to save the active spectrum in the active View under a new filename and/or in a new location.

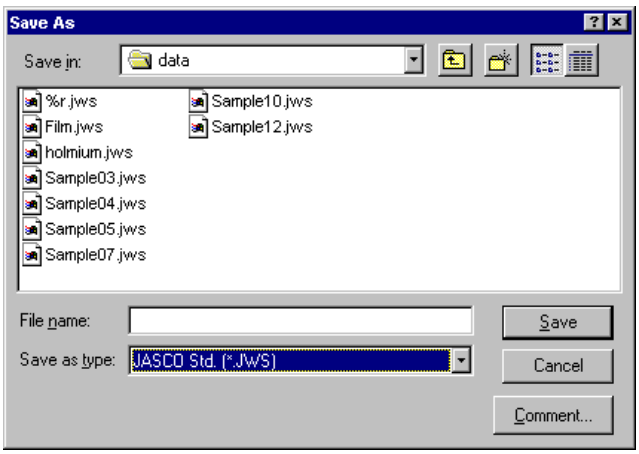


Fig. 2.6 [Save As] dialog box

[Save in] Used to designate the destination drive or directory. Available drives and directories appear in the drop-down list.
The contents of the drive or directory designated in the [Look in] drop-down list are shown in the box below. To use an existing filename click on the desired filename.

[File name] Used to directly input the desired spectrum filename. If the extension is omitted, the designated extension is added automatically. If an existing filename is designated and the <Save> button is clicked, the following dialog box appears.

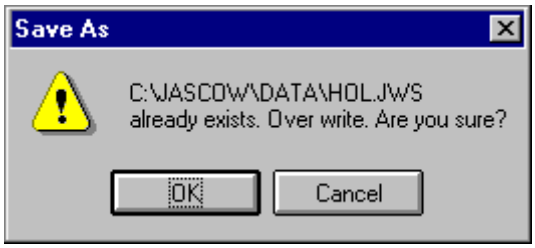


Fig 2.7 Dialog box displayed when an existing filename is designated

Click <OK> to overwrite the contents of the original file.

[Save as type] Lists the available save file types (extensions). If the extension is omitted when the file name is input, the file extension designated here is added automatically.

The following file types can be designated.

Standard data (*.jws): Data measured and calculated using the Spectra Analysis program.

JCAMP-DX_(*.dx): Data in the JCAMP-DX 4.24 format. Refer to the Appendix "JCAMP-DX Format Files" for acceptable formats.

Text File (*.TXT): Data in text format.

<Comment> Click to display the [Comment Edit] dialog box used to enter/edit sample name, operator, organization and comment associated with the file.

2.1.6 [Search...]

Starts the File Find program. Refer to Section 3 “File Find Program” for instructions on how to search for JASCO spectrum files.

2.1.7 [Print...]

Select [File] - [Print...] to print the active View. The spectrum line style, frame, grid, and font, etc are printed according to the designated parameters in [Pattern...], [Font...], and [Style...] in the [View] menu.

If the [Ask the title for printing] box is checked in the [Print] tab of the [Customize] dialog box ([Other] – [Customize…]), when [File] - [Print...] is selected the [Print] dialog box shown below is displayed.

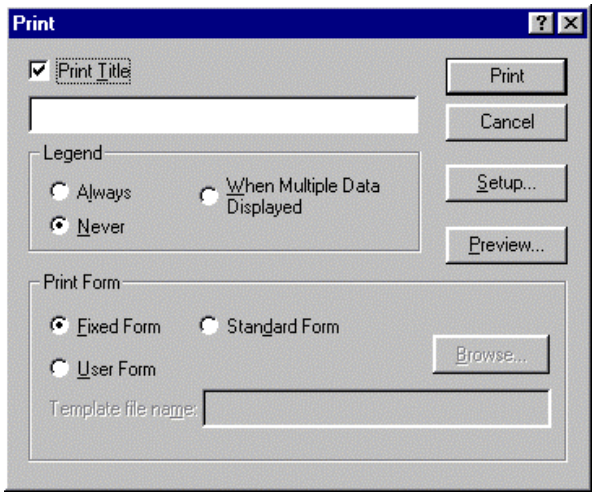


Fig 2.8 [Print] Dialog Box

[Print Title]	Check to print the active view with a title. Enter a title in the text box below.
[Legend] group	Controls whether a legend is printed for spectra.
[Always]	A legend is always printed.
[Never]	A legend spectra is never printed.
[When Multiple Data Displayed]	A legend is printed when two or more spectra are displayed in the active View.
[Print Form] group	Designates the print format.
[Fixed Form]	Select to print using standard format
[Standard Form]	Select to print using the standard format.
[User Form]	Select to print using a template file created in JASCO Canvas. Click the [Browse] button and designate the JASCO Canvas template file to be used.
<Setup>	Opens the [Print Setup] dialog box used to designate the target printer and print parameters.
<Preview>	Shows how the active View will look when printed.

2.1.8 [Print Preview...]

This shows how the active View will look when printed.

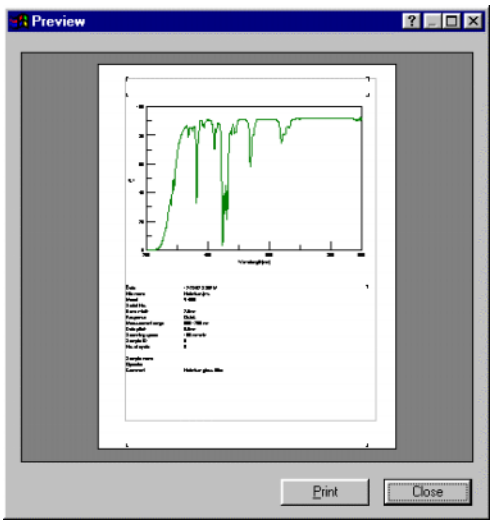


Fig 2.9 [Preview] Dialog Box

<Print> Prints the active View.
<Close> Closes the [Preview] window without printing.

2.1.9 [Print Setup...]

Select [File] - [Print Setup...] to designate the target printer and print parameters.

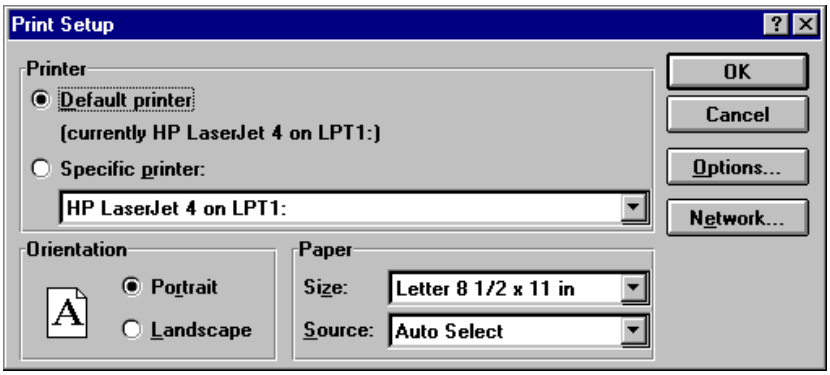


Fig. 2.10 [Print Setup...] Dialog Box

[Printer] group — Click the [Default printer] option button to use the Windows default printer. Click the [Specific printer] option button and select the desired printer from the drop-down list below to use a different printer.

[Orientation] group

[Portrait] — Prints the View so that the short edge of the paper is the top of the page.

[Landscape] — Prints the View so that the long edge of the paper is the top of the page.

[Paper] group

[Size] — Select the paper size from the drop-down list.

[Source] — Select the paper source tray from the drop-down list.

<Options...> — Used to designate parameters for the

target printer. The dialog box that appears differs according to the target printer.

2.1.10 [Exit]

Select [File] - [Exit] to exit the Spectra Analysis program. The following message appears when unsaved spectra exist. To save the spectra, click <Yes>.

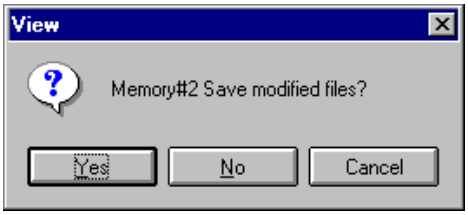


Fig. 2.11 Message displayed when unsaved files exist

<Yes>	Spectra are saved and the Spectra Analysis program ends.
<No>	The Spectra Analysis program ends without saving data.
<Cancel>	Cancels the [Exit] command and returns to the active View.

2.2 [Edit] Menu

This section describes the commands contained in the [Edit] menu.

2.2.1 [Copy Picture]

Select [Edit] - [Copy Picture] to copy a spectrum to the clipboard as a picture. The spectrum can then be pasted into draw-type software such as Microsoft Draw for editing.

2.2.2 [Copy Bitmap]

Select [Edit] - [Copy Bitmap] to copy a spectrum to the clipboard as a bitmap. The spectrum can then be pasted into paint-type software such as Paintbrush for editing. The image becomes distorted if the bitmap is expanded or reduced. Therefore, the size of the window (spectrum) should be adjusted accordingly before copying. A good figure can be obtained if care is taken not to change the ratio between the left and right lengths when reducing later. Expansion always distorts the image.

2.2.3 [Cut Spc.]

Select [Edit] - [Cut Spc.] to remove the currently selected spectrum from the active view and transfer it to the clipboard. When [Select all Spc.] is checked, all the spectra in the active View are cut and the View is closed. Use this command or the [Copy Spc.] command, to place spectra from different Views into one View.

2.2.4 [Copy Spc.]

Select [Edit] - [Copy Spc.] to copy the currently selected spectrum in the active View to the clipboard. The original spectrum remains in the active View. When [Select all Spc.] is checked, all spectra in the active view are copied. Use this command to place spectra from different views into one View.

2.2.5 [Paste Spc.]

Select [Edit] - [Paste Spc.] to paste the contents of the clipboard into the active View.

2.2.6 [Delete Spc.]

Deletes the currently selected spectrum in the active View. When [Select all Spc.] is checked, all spectra in the active view are deleted and the View closes.

Note: When a spectrum is erased, the color of the remaining spectra may change.

2.2.7 [Select all Spc.]

Select [Edit] - [Select all Spc.] to select/deselect all spectra in the active View. When [Select all Spc.] is checked all spectra in the active View are selected. This function can be used in combination with [Cut Spc.], [Copy Spc.] and [Delete Spc.].

2.3 [View] Menu

This section describes the commands contained in the [View] menu.

[Scale...]	Displays the [Scale] dialog box used to change the scale of the spectrum/spectra displayed in the active View.
[Pattern...]	Displays the [Pattern Settings] dialog box used to select the line style and color of the spectrum/spectra displayed in the active View.
[Font...]	Displays the [Font] dialog box used to select the font settings and orientation for the active View.
[Grid...]	Displays the [Grid lines] dialog box used to add/remove vertical and/or horizontal lines to the active View.
[Style...]	Displays the [Scale Setting] dialog box used to change the scale settings for the active View.
[Horizontal Axis...]	Displays the [Horizontal Axis] dialog box used to change the horizontal axis.
[Information...]	Displays spectrum information for the currently selected spectrum in the active View.
[Normalize]	Normalizes the scale of each spectrum displayed in the active View.
[Peak]	Designates how the peak value or peak position of the active spectrum should be displayed when the [Peak Find...] command is executed.

2.3.1 [Scale...]

Select [View] - [Scale...] to display the [Scale] dialog box used to change the scale of the spectrum/spectra displayed in the active View.

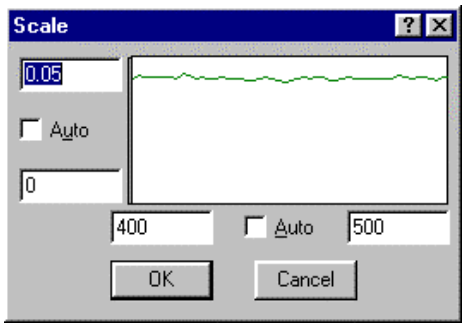


Fig. 2.12 [Scale] dialog box

Horizontal scale	Enter the desired start and end values of the horizontal scale in the text boxes at the bottom of the preview pane. When [Auto] is checked, the input values are ignored and all regions are displayed.
Vertical scale	Enter the desired start and end values of the vertical in the text boxes at the left of the preview pane. When [Auto] is checked, the input values are ignored and the most appropriate scale for the designated horizontal range is displayed.

2.3.2 [Pattern...]

Select [View] - [Pattern...] to display the [Pattern Settings] dialog box used to select the line style and color of the spectrum/spectra displayed in the active View.

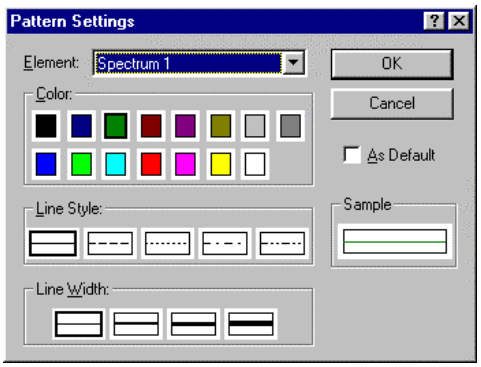


Fig. 2.13 [Pattern Settings] dialog box

[Element]	Lists items for which the color or line style can be changed.
[Color]	Shows available colors. Select desired color from this palette. The currently designated item in the [Element] list is displayed in the selected color.
[Line Style]	Shows available line styles. The currently designated item in the [Element] list is displayed with the selected line style.
[Line Width]	Shows available line widths. The currently designated item in the [Element] list is displayed with the selected line width.
[Sample]	Displays a sample of the designated pattern.
[As Default]	Check to use the designated pattern for all subsequently opened views.

2.3.3 [Font...]

Select [View] - [Font...] to display the [Font] dialog box used to select the font settings and orientation for the active View.

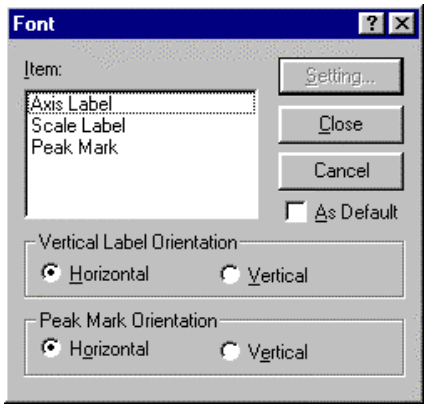


Fig. 2.14 [Font] dialog box

[Item]	Lists the items for which the font settings can be changed. The font settings for the axis label, scale label, and peak mark can all be changed.
<Setting...>	Click to change the font settings for the currentl designated [Item].
[Vertical Label Orientation] group	Sets the label orientation for the vertical axis.
[Peak Mark Orientation] group	Sets the label orientation for the peak mark.
[As Default]	Check to use the designated font settings for all subsequently opened views.

2.3.4 [Grid...]

Select [View] - [Grid] to display the [Grid lines] dialog box used to add/remove vertical and/or horizontal lines to the active View.

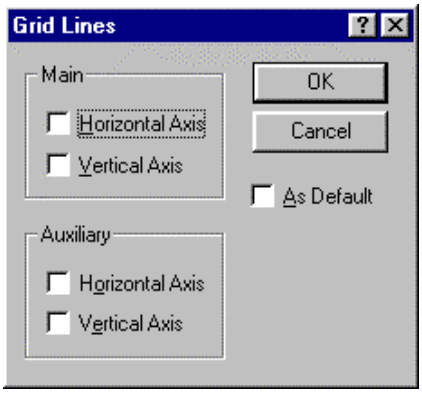


Fig. 2.15 [Grid Lines] dialog box

[Main] group
- [Horizontal Axis] Check to display main horizontal axis lines.
- [Vertical Axis] Check to display main vertical axis lines.

[Auxiliary] group
- [Horizontal Axis] Check to display auxiliary horizontal axis lines.

[Vertical Axis] Check to display auxiliary vertical axis lines.
[As Default] Check to use the current grid lines for all subsequently opened views.

Note: When the [Apply view setting to all spectra] check box in the [Customize] dialog box is checked, the grid lines settings are applied to all Views.

2.3.5 [Style...]

Select [View] - [Style...] to display the [Scale Setting] dialog box used to change the scale settings for the active View.

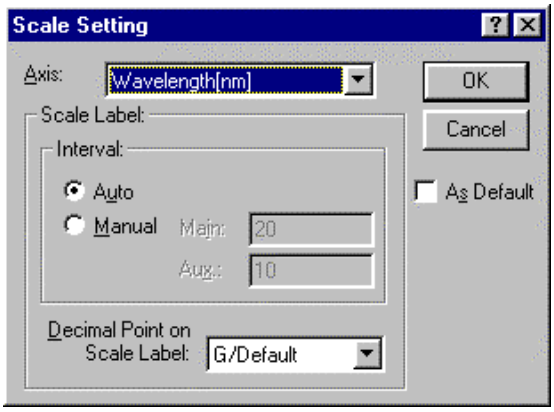


Fig. 2.16 [Style Setting] dialog box

[Axis] Lists the available formats for the horizontal and vertical axis.

[Interval] group

[Auto] Select the [Auto] option button to automatically designate the grid format.

[Manual] Select the [Manual] option button to manually set the grid format of the main and auxiliary scale.

[Decimal Point on scale label] Designates the number of decimal places for the horizontal and vertical axis display values.

[As Default] Check to use the current scale settings for all subsequently opened views.

2.3.6 [Horizontal Axis...]

Select [View] - [Horizontal Axis...] to display the [Horizontal Axis] dialog box used to change the horizontal axis.

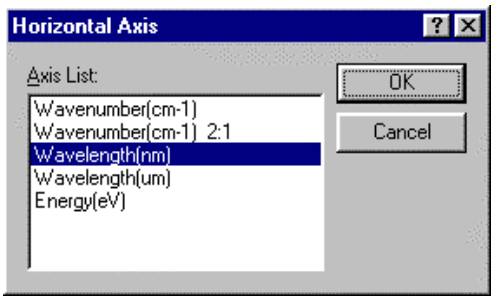


Fig. 2.17 [Horizontal Axis] dialog box

[Axis List] Lists the available formats for the horizontal axis.

2.3.7 [Information...]

Displays spectrum information for the currently selected spectrum in the active View.

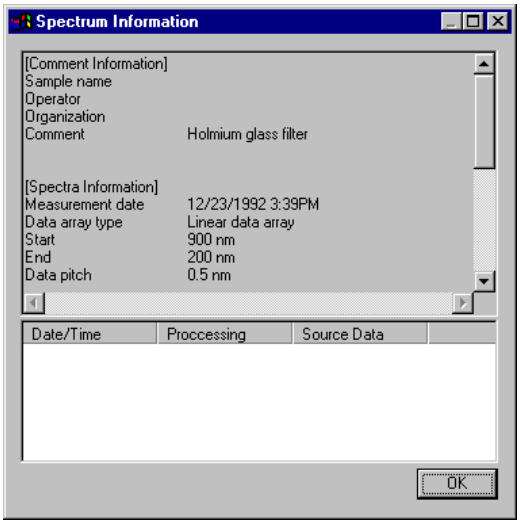


Fig 2.18 [Spectrum Information] dialog box

2.3.8 [Normalize]

Automatically normalizes the scale of each spectrum displayed in the active View. The purpose of this function is so that spectra with different vertical axis scales can be viewed at the same time in a single View window. When the [Normalize] function is active, a box appears around the vertical axis label in the active View.
For example, for two spectra displayed in %T mode and Abs mode, the spectrum displayed in Abs mode is not visible as shown in Fig. 2.19.

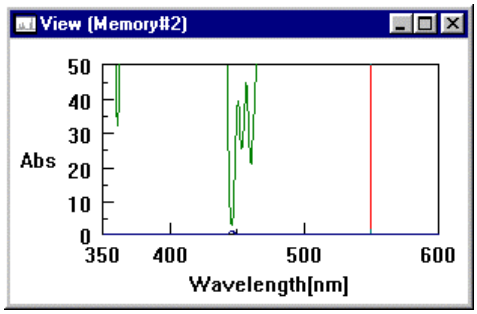


Fig 2.19 Overlay - View

By switching to [Normalize] both spectra are visible as shown in Fig. 2.20.

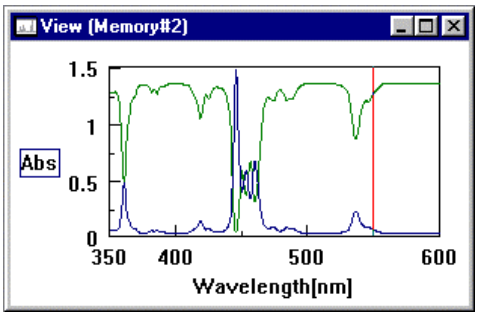


Fig 2.20 Normalize - View

2.3.9 [Peak]

Click [View] - [Peak] to display a submenu in which you can designate how the peak value or peak position of the active spectrum should be displayed when the [Peak Find...] command is executed.

[None]	Peak position not displayed.
[Bar]	Denotes peak position with a vertical bar.
[Bar, Data No.]	Denotes peak position with a vertical bar, and displays the peak number.
[Bar, X]	Denotes peak position with a vertical bar, and displays the horizontal axis value.
[Bar, Y]	Denotes the peak position with a vertical bar, and displays the vertical axis value.
[Bar, X, Y]	Denotes the peak position with a vertical bar, and displays the horizontal and vertical axis values.

2.3.10 [Legend display switcing]

Switches over the legend display of active view spectrum in the spectral analysis window. A legend is displayed in the tool bar if the tool button  is not clicked (see Fig. 2.24 (a)). Clicking the tool button  displays a legend on the status bar (see Fig. 2.24 (b)). In addition to the filename are displayed measurement date, sample name, operator's name, organization and comment. O before the filename is green if the spectrum is saved or red if not.  before the filename is green if the spectrum is saved or red if not.

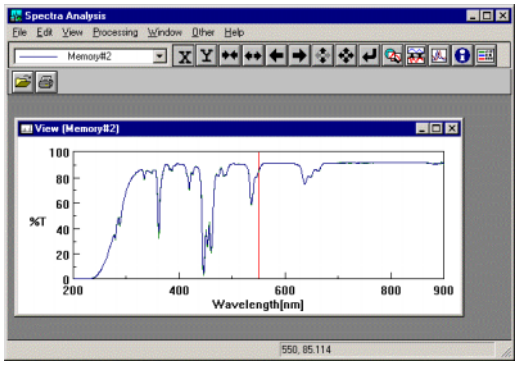


Fig. 2.24 (a) Display of legend on tool bar

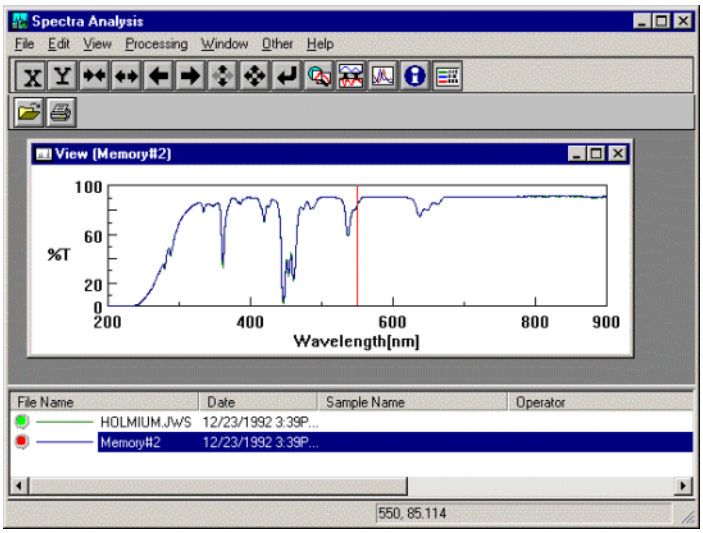
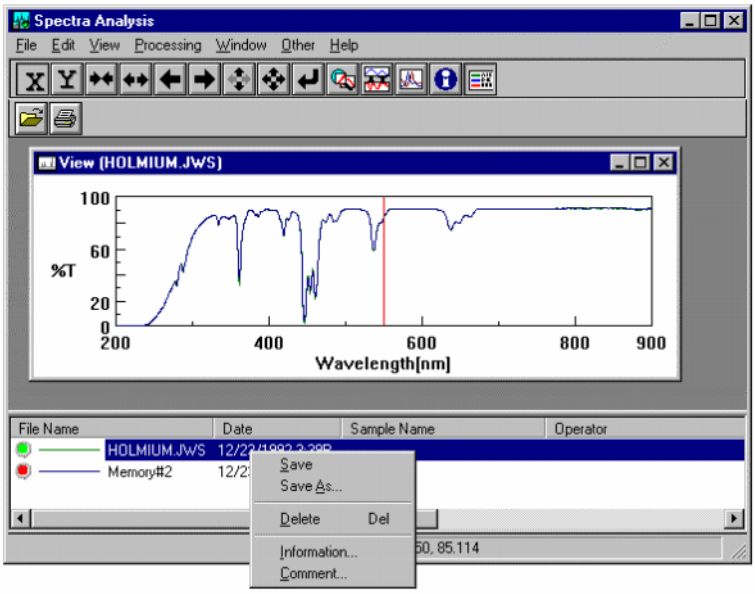
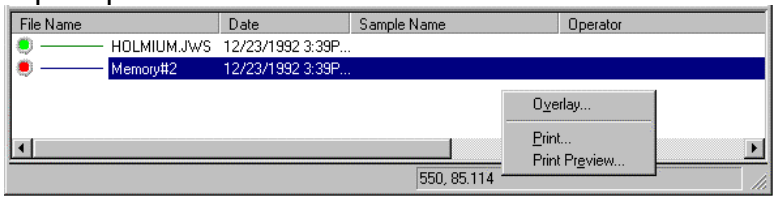


Fig. 2.24 (b) Display of legend on status bar

Double-clicking the legend filename displayed on the status bar allows the spectrum to be saved by assigning a name to it. Double-clicking the measurement date displays spectrum information, and double-clicking the sample name, operator's name, organization or comment opens the comment edit dialog, allowing the sample name, operator's name, organization and comment to be edited.
Spectra can be overlaid in an active view by double-clicking a location where legend is not displayed.
Also right-clicking each legend displays the menu for save, save as, delete spectrum, spectrum information or edit comment.



Right-clicking a location where legend is not displayed displays the menu for overwrite, print, or print preview.



2.4 [Processing] Menu

This section describes the commands contained in the [Processing] menu.

[Correction] submenu

[Baseline...]	Displays the [Baseline Correction] dialog box used for correcting a spectrum using a free baseline.
[Smoothing...]	Displays the [Smoothing] dialog box used to smooth spectrum data.
[Noise Elimination...]	Displays the [Noise Elimination] dialog box used to eliminate pseudo-peak(s) caused by noise or some other known cause.
[Deconvolution...]	Displays the [Deconvolution] dialog box used to analyze bands that may contain overlapping Lorentzian curves having the same FWHM values and accurately distinguishes the peak positions for each band.
[FFT filter...]	Displays the [FFT Filter] dialog box used to separate a spectrum into frequency components using a Fast Fourier Transformation. Eliminates noise having a particular periodicity.
[Data Cut...]	Displays the [Approximate and Data Cut] dialog box used to create a spectrum with an arbitrary data interval in an arbitrary wavelength region. Data in any wavenumber region can also be cut without changing the data.

[Operation] submenu

[Arithmetic...]	Displays the [Arithmetic] dialog box used to perform arithmetic operations between spectra or between a spectrum and a constant.
[Derivatives...]	Displays the [Derivatives] dialog box used to obtain the 1st, 2nd or 3rd order derivative of a spectrum.
[KK conversion...]	Displays the [KK Conversion] dialog box used to correct the specular reflection spectrum (Kramers-Kronig conversion).

[Peak Process] submenu

[Peak Find...]	Displays the [Peak Find] dialog box used to find spectrum peaks and/or valleys.
[Peak Height...]	Displays the [Peak Height] dialog box used to determine peak height and height ratio.
[Peak Area...]	Displays the [Peak Area] dialog box used to determine peak area and area ratio.
[Peak Width...]	Displays the [Peak Width] dialog box used to calculate the full width at half maximum value.
[Subtraction...]	Displays the [Subtraction] dialog box used to determine a difference spectrum.
[X Unit Conversion...]	Displays the [X Unit Conversion] dialog box used

	to convert the X-axis units of the active spectrum.
[Y Unit Conversion...]	Displays the [Y Unit Conversion] dialog box used to convert the Y-axis units of the active spectrum.

[Other...] submenu

[Comment...]	Displays the [Comment Edit] dialog box used to add or edit comments.

[Common Options] submenu

[Kinetics...]	Displays the [Kinetics] dialog box used to calculate an enzyme activity value.
[Data Dump…]	Displays the [Data Dump Parameter] dialog box used to display measured data values and copy them to the clipboard.
[Arithmetic with Data...]	Performs arithmetic operations using data overlaid in the same channel of a view.
[Arithmetic with Channel...]	Performs arithmetic operations using data freely selected from multiple channels of data displayed in a view.
[Move Channel…]	Moves channels in a view or picks up only data of a desired channel from data overlaid in a view or from multiple-channel data.
Data Accumulation	Accumulates the data overlaid in the same channel of a View and displays the accumulated data in a new View.

[CD Options] submenu

[HT -> OD…]	Converts HT voltage data to absorbance.
[Optical Constant…]	Calculates optical constants.
[KK Conversion…]	Converts CD data to ORD or ORD data to CD.
[G-value…]	Calculates the G value which represents the degree of asymmetry of the absorption band.
[pH conversion]	Opens a new view with CD value (or fluorescence, HT or other) displayed on the vertical axis and pH data on the horizontal axis

[FP Options] submenu

[Phospho. Lifetime...]	Displays the [Phosphorescent Lifetime Analysis] dialog box used to calculate phosphorescent lifetime.

[IR Options] submenu

[ATR conversion…]	Converts the absorption intensity relationship between the high wavenumber side and low wavenumber side.
[IF to spectrum…]	Converts an intrferogram(IF) into a single-beam spectrum.
[Spectrum to IF…]	Converts a single-beam spectrum into an interferogram(IF).

2.4.1 [Correction] submenu

2.4.1.1 [Baseline...]

Select [Processing] - [Correction] - [Baseline...] to correct the active spectrum using a free baseline. A baseline with a maximum of 32 variable points (including both ends) can be created. The variable points can be connected with a straight line or a spline curve.

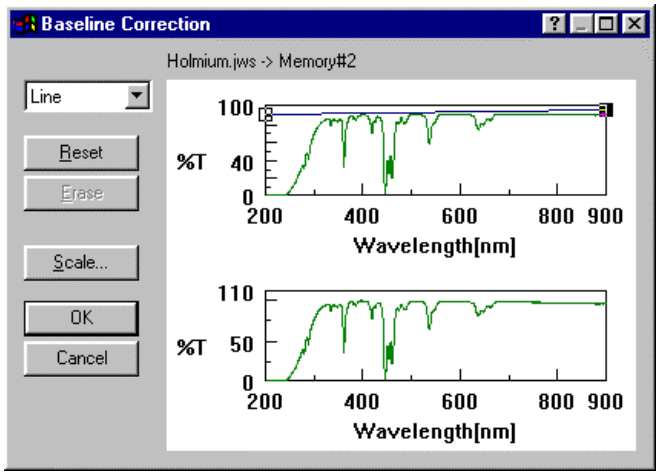


Fig. 2.21 [Baseline Correction] dialog box

Baseline drop-down list

[Line]	Select to connect adjacent variable points with a straight line.
[Spline]	Select to connect adjacent variable points with a spline curve.
<Reset>	Click to restore the baseline to its original shape (i.e. two variable points connected with a straight line).
<Erase>	Click to erase a single variable point. Darkened points or points with thick square frames can be erased. If a variable point on the left or right end is erased, the next point becomes the end point.
Spectrum display area	Set the spectrum baseline in the upper spectrum to display the results below. Move the small squares on the baseline (initially only at the ends) to change the baseline shape. When the pointer approaches a square, the shape of the pointer changes to a set of tweezers that can be used to drag the square to another location. When the pointer approaches the baseline, the shape of the pointer changes to a syringe. Click the left mouse button to add variable points.

2.4.1.2 [Smoothing...]

Select [Processing] - [Correction] - [Smoothing...] to smooth the active spectrum. The following four methods are available: Means-Movement, Savitzky-Golay, Adaptive-Smoothing and Binomial.

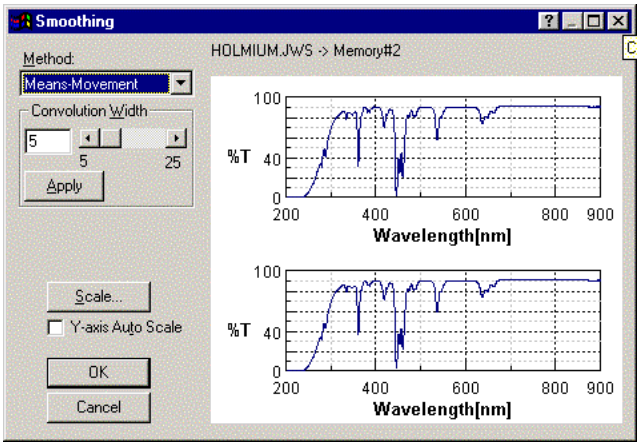


Fig. 2.22 [Smoothing] dialog box

[Method] drop-down list	Lists available smoothing methods.
[Convolution Width]	Sets the number of data points to be bundled on both sides for each data point. Only odd numbers can be set. Values are immediately recalculated after each change.
<Apply>	Applies the set convolution width value, and then calculates.
Spectrum display area	The original spectrum is displayed at the top, the smoothed spectrum below.
<Scale...>	Click to set the spectrum range.
[Y-axis Auto Scale]	Check this box to view the results using the auto scale function. Deselect when viewing the change in the size of the differential spectrum.

Note: Refer to "Smoothing Method" in the Appendix for details of each method.

2.4.1.3 [Noise Elimination...]

Select [Processing] - [Correction] - [Noise Elimination...] to eliminate false peaks due to noise of known origin. The peak is eliminated by connecting the designated horizontal axis ranges with a straight line. The horizontal axis range can also be changed.

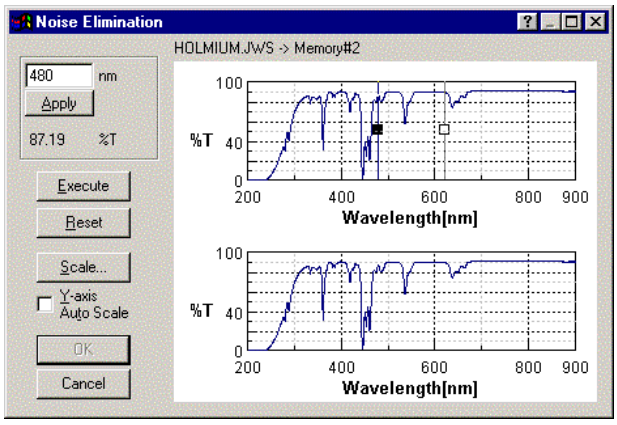


Fig. 2.23 [Noise Elimination] dialog box

Wavelength display	Displays the position of the active wavelength axis setting bar. Input a wavelength, and then click <Apply> to shift the active wavelength setting bar to the designated position.
<Apply>	Moves the active wavelength setting bar to the designated position.
<Execute>	Executes noise elimination.
<Reset>	Resets the spectrum to its original condition before noise elimination.
Spectrum display area	The original spectrum is displayed at the top, and the spectrum with noise removed below.
<Scale...>	Click to set the spectrum range.
[Y-axis Auto Scale]	Check this box to view the results using the auto scale function. Deselect when viewing the change in the size of the differential spectrum.

2.4.1.4 [Deconvolution...]

This function analyzes bands that may contain overlapping Lorentzian curves having the same full width at half maximum value and accurately distinguishes the peak positions for each band.

Note: The region outside the wavelength range of interest will also be influenced by the deconvolution calculation, and the spectral profile will change.

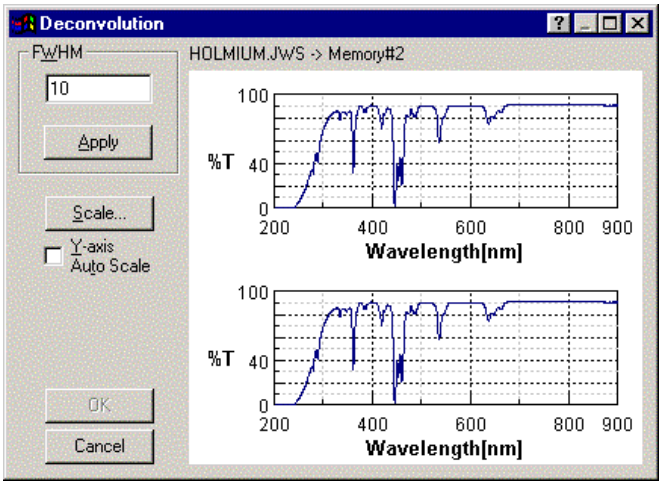


Fig. 2.24 [Deconvolution] dialog Box

Note: Figure 2.24 shows spectra before execution of deconvolution, therefore, the upper and lower spectra in the spectrum display area are the same. After execution, the resulting spectrum is displayed in the lower half of the spectrum display area.

[FWHM]	Specify the full width at half maximum value of the expected Lorenz waveform.
<Apply>	Click to perform deconvolution using the input value.
<Scale...>	Click to set the spectrum range.

[Y-axis Auto Scale] Check this box to view the results using the auto scale function. Deselect when viewing the change in the size of the differential spectrum.

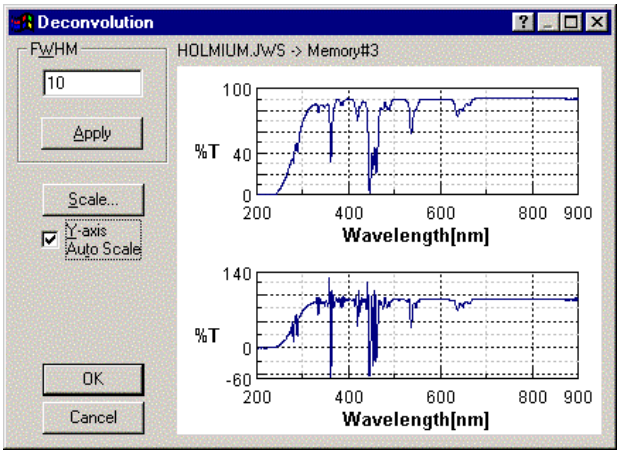


Fig 2.25 [Deconvolution] result screen (example)

Note: Before clicking <OK> and confirming the changes, you can execute deconvolution with different full width at half maximum values as many times as you wish. The results are displayed in the lower half of the spectrum display area. For more details on deconvolution refer to the Appendix.

2.4.1.5 [FFT filter...]

Separates the spectrum into frequency components using a Fast Fourier transformation and eliminates noise having a particular periodicity. A filter containing a maximum of 32 variable points (including both ends) can be created. However, if the peaks and noise are almost the same height, the noise cannot be removed.

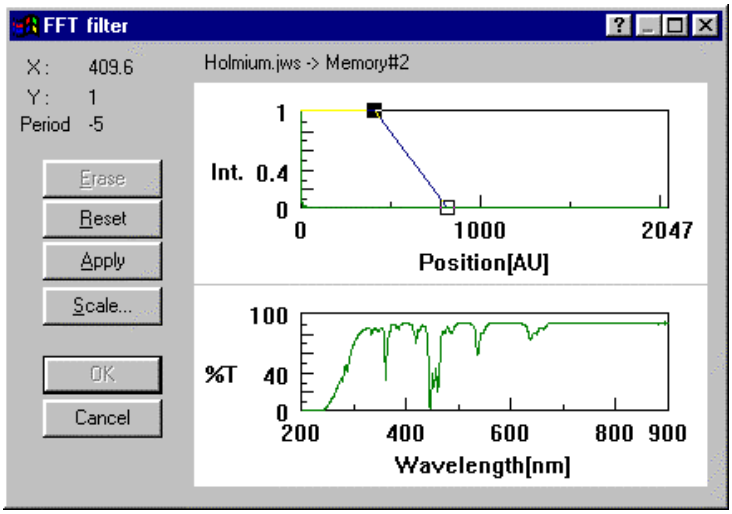


Fig. 2.26 [FFT filter] dialog box

Note: Figure 2.26 shows spectra before execution of FFT filter, therefore, the upper and lower spectra in the spectrum display area are the same. After execution, the resulting spectrum is displayed in the lower half of the spectrum display area.

Spectrum display area	Set the shape of the FFT filter in the upper spectrum and the results are displayed below. Move the small squares on the filter (initially only at the ends) to change the shape. When the pointer approaches a square, the shape of the pointer changes to a set of tweezers that can be used to drag the square to another location. When the pointer approaches the filter, the shape of the pointer changes to a syringe. Click the left mouse button to add variable points. The X and Y values at the left correspond to the coordinates of the variable point and the period to the period of noise (nm).
<Erase>	Click to erase a single variable point. Darkened points or points with thick square frames can be erased. If a variable point on the left or right end is erased, the next point becomes the end point. The minimum number of variable points is two. If only two points exist, neither can be erased.
<Reset>	Returns the filter to its original shape.
<Apply>	Click to perform calculation with the set filter. The resulting spectrum is displayed in the lower half of the spectrum display area.

2.4.1.6 [Data Cut...]

Creates a spectrum with an arbitrary data interval in an arbitrary region of the X-axis. Data in any region of the X-axis can also be cut without changing the data.

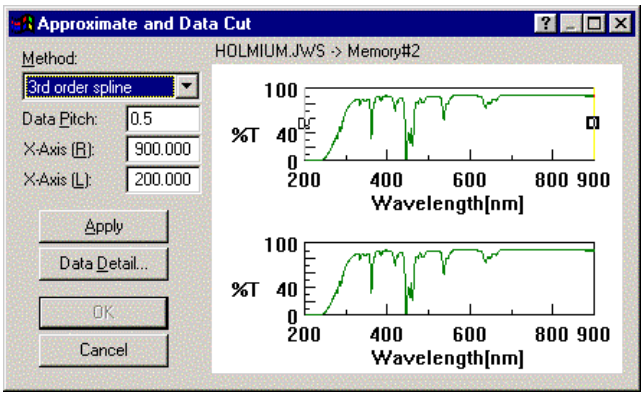


Fig 2.27 [Approximate and Data Cut] dialog box

Note:	*Figure 2.27 shows spectra before execution of data interpolation and cut, therefore, the upper and lower spectra in the spectrum display area are the same. After execution, the resulting spectrum is displayed in the lower half of the spectrum display area.*

Spectrum display area	The original spectrum is displayed at the top, and the spectrum with noise removed below.
[Method] drop-down list	Select the method of data interpolation. The following options are available (see reference section below):

	[Lagrange]	Lagrangian interpolation
	[3rd order spline]	Tertiary spline interpolation
	[No correction]	Select this when cutting data.
[Data pitch]	Specify the pitch of the data to be created.	
[X-Axis (L)]	Specify the lower X-axis value of the data to be created.	
[X-Axis (R)]	Specify the upper X-axis value of the data to be created.	
<Apply>	Click to execute data interpolation and cut using the entered values.	
<Data Detail>	Click to display information for the original spectrum.	

Note: The resulting spectrum data can be saved in text file format to be utilized in other applications.

Reference: Methods of data interpolation

Data interpolation determines the interpolation function, F that satisfies $Y_i = (X_i)$; i=1,2,3,... N from the data points $\{(X_i,Y_i)$; i=1,2,3,...N$\}$ obtained by measurement in order to estimate Y with respect to X (except for known X_i).

"Lagrange interpolation" and "Tertiary spline interpolation" are representative methods of data interpolation.

(1) Lagrange interpolation

This method determines a function F that passes all data points in a specified range for interpolation. For N data points, the interpolation function F is basically an $(N - 1)^{th}$ function, thus making it complicated. However, in practice, calculation is made by making some contrivances.

(2) Tertiary spline interpolation

This method calculates the values between N data points within a specified range by using (N - 1) items of different tertiary functions F_i. The interpolation functions F_i and F_i+1 of adjacent sections are determined so that the value of the function and the primary and secondary derivative factors at the boundary point agree with each other.

2.4.2 [Operation] submenu

2.4.2.1 [Arithmetic...]

Select [Processing] - [Operation] - [Arithmetic...] to perform an arithmetic operation between spectra or between a spectrum and a constant(s). When only one spectrum is displayed in the active view, the arithmetic operation is performed using a constant(s). When two or more spectra are displayed, the arithmetic operation is performed between the spectra. When three or more spectra are displayed, The spectra used for arithmetic operation must be designated from the [Select Spectrum] dialog box which opens before the [Arithmetic] dialog box.

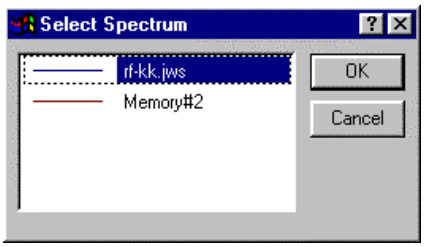


Fig. 2.28 [Select Spectrum] dialog box

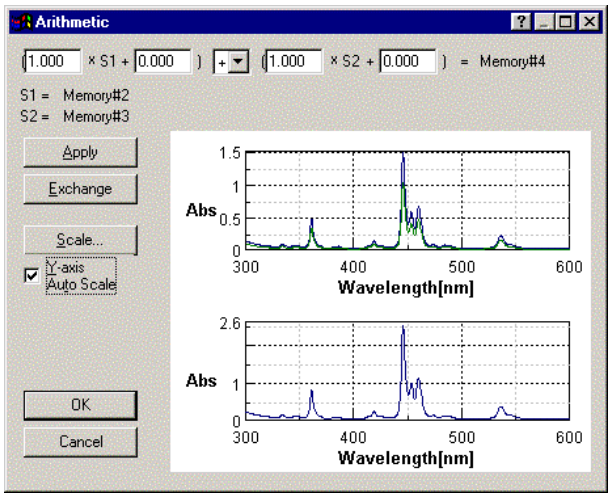


Fig. 2.29 [Arithmetic] dialog box (when two spectra are displayed)

The operation to be performed is shown at the top of the dialog box. S1 and S2 represent the selected spectra and are defined below. Enter constants into the appropriate text boxes and select the desired arithmetic operator from the drop-down list to generate an arithmetic expression.

<Apply>	Click to execute calculation using the designated parameters.
<Exchange>	Reverses the positions of spectra S1 and S2.
Spectrum display area	The original spectrum or spectra is (are) displayed at the top, the results of the arithmetic operation below.
<Scale...>	Click to set the spectrum range.
[Y-axis Auto Scale]	Check this box to view the results using the auto scale function. Deselect when viewing the change in the size of the differential spectrum.

Note: To perform arithmetic operation between one spectrum and a constant in a view in which multiple spectra are displayed, open the dialog according to the same procedure as when performing an arithmetic operation between two spectra. Input 0 for the factor and a constant not related to the operation.

Note: The result of dividing between single beams (SB) is converted to %T. When adding or subtracting %T (%R), the values are added or subtracted in the same units. (Addition of 100% and 100% makes 200% and subtraction becomes 0%. (This is in contrast to the difference spectrum obtained using "difference by conversion to ABS.")

2.4.2.2 [Derivatives...]

Select [Processing] - [Operation] - [Derivatives...] to determine the derivative of a spectrum. First-, second-, and third-order derivative calculations can be performed.
Differentiates spectrum. Can be selected from [Subtract] and [Savitzky-Golay method].

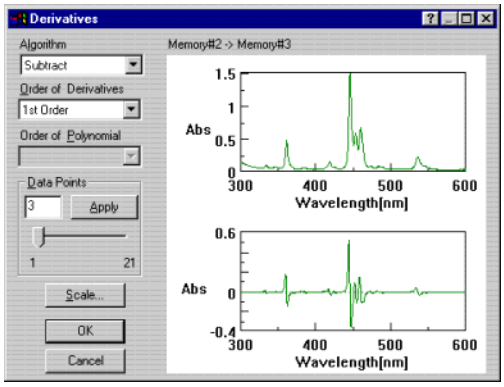


Fig. 2.30 [Derivatives] dialog box

[Algorithm]	Selects the derivative system from the drop-down list.
[Order of Derivatives]	Select the order of the derivative.
[Order of Polynomial]	Selects the order of polynomial by [Savitzky-Golay method].
[Data Points]	Selects the interval between data points.

Note: In the derivatives of a spectrum containing high noise, it is recommended to conduct smoothing first or use a higher number of [Data Points].

2.4.2.3 [KK Conversion...]

This function is used to determine the absorbance from a specular reflection spectrum (Kramers-Kronig conversion). Only available for spectra for which the vertical axis is absorbance (Abs), %T or %R.
Since the specular reflection spectrum is affected by the refractive index and absorption of the sample, the spectrum is measured using a derivative profile. The derivative profile can be divided into two components: an absorption index(k) and a refractive index(n), by subjecting it to Kramers-Kronig conversion. This processing can be used effectively for a spectrum with a derivative profile and for which both ends are flat. In addition, when applying Kramers Kronig conversion to only a specific region, select a region for which both ends are flat.

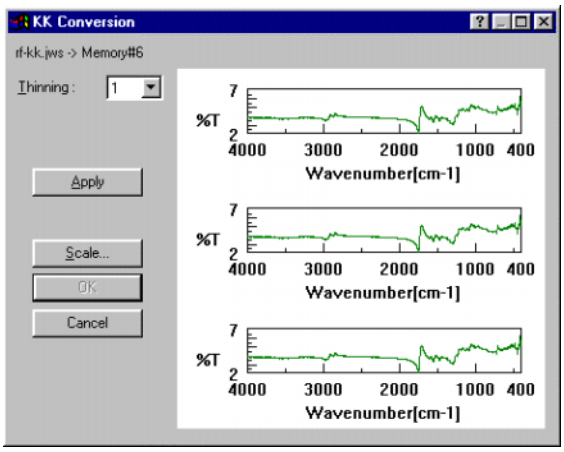


Fig 2.31 [KK Conversion] dialog box

Note: Figure 2.31 shows spectra before execution of KK conversion, therefore, all three spectra in the spectrum display area are the same. After execution, the top spectrum is the original spectrum, the middle spectrum is the KK-converted spectrum and the bottom spectrum is the refractive index spectrum obtained through calculation.

Spectrum display area	The top spectrum is the original spectrum, the middle spectrum is the KK-converted spectrum and the bottom spectrum is the refractive index spectrum obtained through calculation.
[Thinning]	Designates the interval between data points to be used for calculation. Calculation is faster when this value is large.
<Apply>	Click to execute calculation using the set parameters. The KK-converted spectrum is in Abs mode.
<OK>	Click to close the dialog box. Two Views containing the absorption index(k) spectrum and refractive index(n) spectrum are displayed.

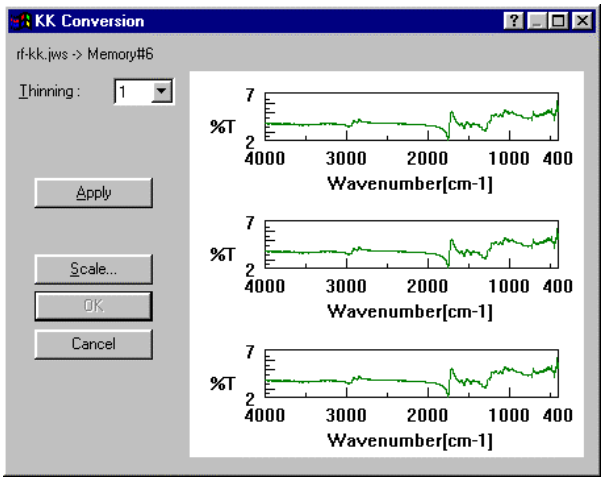


Fig 2.32 [KK Conversion] result dialog box

2.4.3 [Peak Process] submenu

2.4.3.1 [Peak Find...]

Select [Processing] - [Peak Process] - [Peak Find...] to display the [Peak Find] dialog box used to detect spectrum peaks/valleys. A maximum of 100 peaks/valleys can be detected for each spectrum.

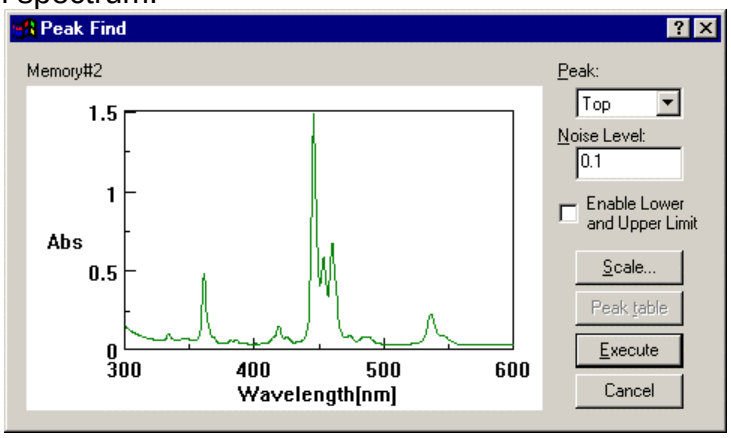


Fig. 2.33 [Peak Find] dialog box

[Peak] drop-down list	Lists available modes for detecting peaks/valleys. Top: Detects peaks. Bottom: Detects valleys. Both: Detects both peaks and valleys.
[Noise Level]	Enter a threshold value used to recognize a peak/valley. When the difference between the start of a peak/valley to its apex does not meet or exceed this value, the peak will not be recognized. The units are the same as those used in the active spectrum.
[Enable Lower and Upper Limit]	When this box is checked the peak find function searches the portion of the spectrum currently displayed in the dialog box, in other words, within the limits of the x- and y-axes. Therefore, by changing the scale settings it is possible to search within a specific region of the measured spectrum. When this box is unchecked the peak find function searches the portion of the spectrum contained within the limits of the current x-axis and ignores the limits of the y-axis.
<Peak table>	Click to display a table of the previous peak find results for the active spectrum. This display is the same as that which appears when <Execute> is clicked and peaks/valleys are found.
<Execute>	Click to find peaks and/or valleys. The dialog box closes and the results of the search are displayed.

The following explains the components of the [Peak Find] results dialog box.

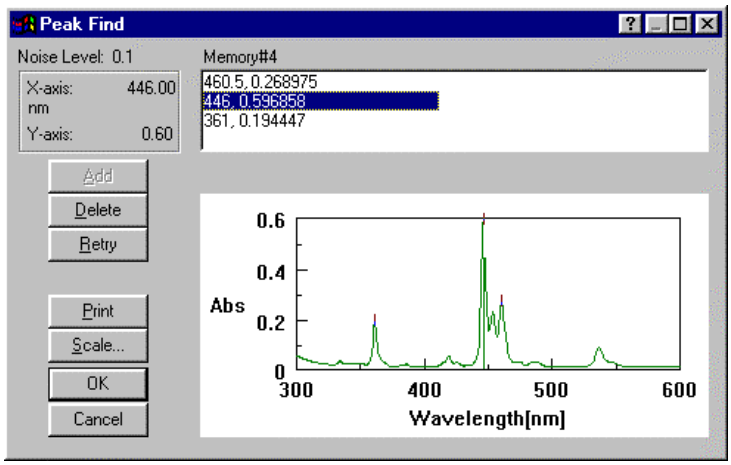
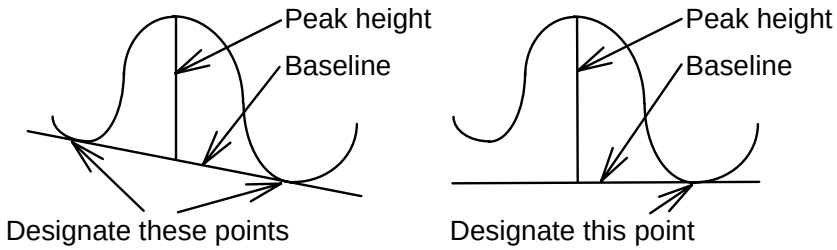


Fig. 2.34 [Peak Find] results dialog box

Peak list	Displays the peak find results for the active spectrum. Clicking on a value causes a vertical line to appear at the selected peak/valley position in the spectrum display area below. The peak/valley position and intensity are displayed as X- and Y-axis values, respectively, in the box to the left.
Spectrum display area	By clicking on the short bar that indicates a peak position, the long bar will move to that position. The selected value in the peak list becomes highlighted. This operation is the same as clicking on a value in the peak list. The long bar can also be moved to locations other than peak/valley positions by clicking the desired position in the spectrum. The wavelength and Abs for the position appear against the X- and Y-axis, respectively, in the box to the left. To add a peak, click on the desired peak position, and then click <Add>.
<Add>	Click to add a peak. Click <Add> after clicking on the desired position.
<Delete>	Click to delete a peak. Select the peaks to be deleted in the peak list or in the spectrum display, and then click.
<Retry>	Click to stop operation and return to the previous dialog box.
<Print>	Click to open the [Print] dialog box. For details refer to Section 2.1.7.

2.4.3.2 [Peak Height...]

This function detects the peak height and calculates the height ratio. Two methods are available for finding the peak height.



(1) 2 Point base: Designate 2 points to determine the baseline

(2) 1 Point base: Designate 1 point to determine the baseline

Fig. 2.35 Methods for finding peak height

The [Peak Height] dialog box contains parameters for detecting the peak height and calculating the height ratio. Since the [Peak Height] dialog box contains many elements, before explaining each element in the dialog box the procedure for calculating peak height is described below.

The following example explains how to automatically detect a peak using the [2-Point Base] method.

(1) Select [Processing] - [Peak Process] - [Peak Height...] to display the following dialog box.

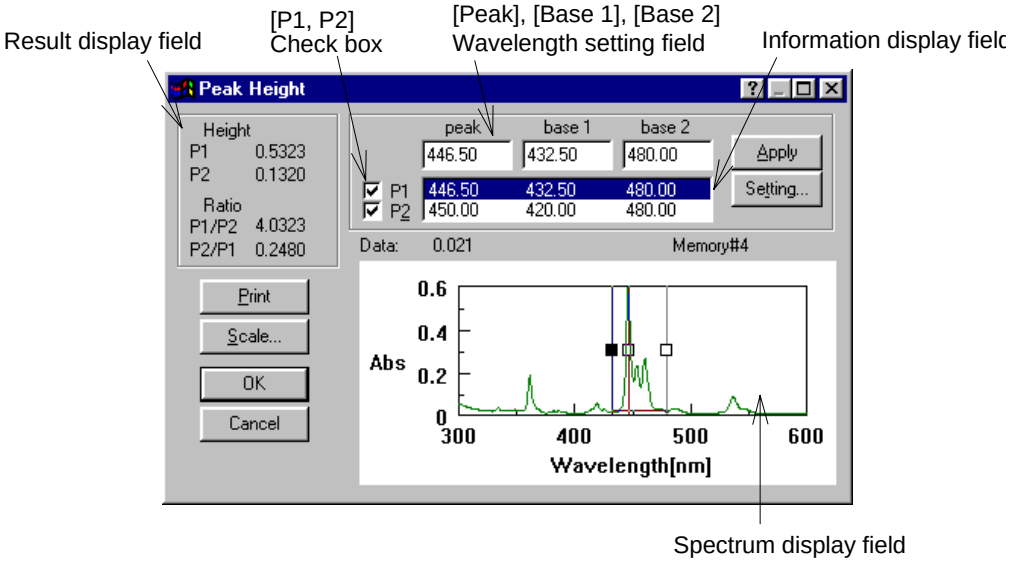


Fig. 2.36 [Peak Height] dialog box

(2) Check the [P1] checkbox to calculate the peak height.

Note: [P2] should also be selected when calculating the peak height ratio.

(3) Click <Setting...> to open the [Peak Height - Set] dialog box. Set the peak height detecting parameters as follows.

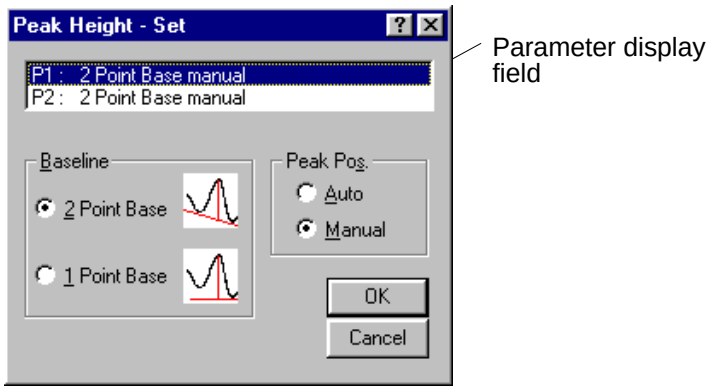


Fig. 2.37 [Peak Height - Set] dialog box

(a) Click on [P1] in the parameter display field to set the parameters for [P1].
(b) Select the [2 Point Base] option button in the [Baseline] group.
(c) Select the [Auto] option button in the [Peak Pos.] group.

Note:	*When calculating the peak ratio, repeat steps 3a) to 3c) replacing [P1] for [P2] to set the parameters for [P2].*

Click <OK> to close the [Peak Height - Set] dialog box.

(4) Set the base wavelength for Peak 1 as follows.
(a) Click on the row of numbers to the right of [P1] in the information display. The wavelengths of peak [P1] and the base position are displayed in the wavelength setting fields, allowing the wavelength to be changed.
(b) Set the base wavelength using the wavelength setting bar on the spectrum. The wavelength can also be set by directly inputting a value into the text box, and then clicking <Apply>. Peak height is calculated and displayed in the result display field.

Note:	*When calculating peak ratio, set the wavelength for Peak 2 using the same procedure.*

(5) Click [Print] to open the [Print] dialog box. Click <OK> to print the results.

[Peak Height] dialog box

Result display field:	When the [P1] and [P2] checkboxes are selected, the heights of P1 and P2 are displayed at [P1] and [P2], respectively, and the height ratios of Peak 1/Peak 2 and Peak 2/Peak 1 are displayed at [P2/P2] and [P2/P1], respectively. The results are recalculated and redisplayed each time the peak and base wavelength are changed.
[P1], [P2]	Check these boxes to display the calculation results in the Result display fields.
[Peak], [Base 1], [Base 2]	Wavelength setting fields for Peak 1, Base 1 and Base 2.
Information display field:	Displays the peaks and base wavelength of [P1] and [P2] for calculating the peak height/height ratio. Click the

	wavelength setting box to change the wavelength using the wavelength setting bar.
Spectrum display area	Set the peak or base wavelength by dragging the wavelength setting bar on the spectrum. The peak height/height ratio is calculated at the same time as it is set. The data of the active wavelength setting bar appears at the upper-right side of the display beside [Data].
<Apply>	After entering the Peak, Base 1 and Base 2 values, click <Apply> to move the wavelength setting bar to the designated wavelengths and execute calculation.
<OK>	Closes the dialog box and stores the peak height information in memory.
<Print>	Opens the [Print] dialog box. For details refer to Section 2.1.7.
<Setting...>	Click to open the parameter setting dialog box for calculating the peak height and peak height ratio.

[Peak Height-set] dialog box

Parameter display field:	Displays the [P1] and [P2] calculation parameters. Click on [P1] to set the parameters for [P1]. Similarly, for [P2].
[Baseline] group	Contains the available baseline drawing methods.
[2 Point Base]	Draws baseline by designating two points.
[1 Point Base]	Draws baseline in the horizontal direction by designating one point as a reference.
[Peak Pos.] group	Select either [Auto] detection or [Manual] setting of peak position. For [2 Point Base], [Auto] setting recognizes the position where absorption is highest as the peak within the range designated by Base 1 and Base 2. For [1 Point Base], [Auto] cannot be designated.
<OK>	Closes the dialog box and returns to the [Peak Height] dialog box.

2.4.3.3 [Peak Area...]

This function determines the peak area and calculates the area ratio. Three methods are available for determining the peak area:

(1)	[2 Point Base]	Determines total area within baseline
(2)	[No Base]	Assumes 0 or 100% as the baseline
(3)	[Arbitrary Base]	Sets the baseline and peak ranges separately

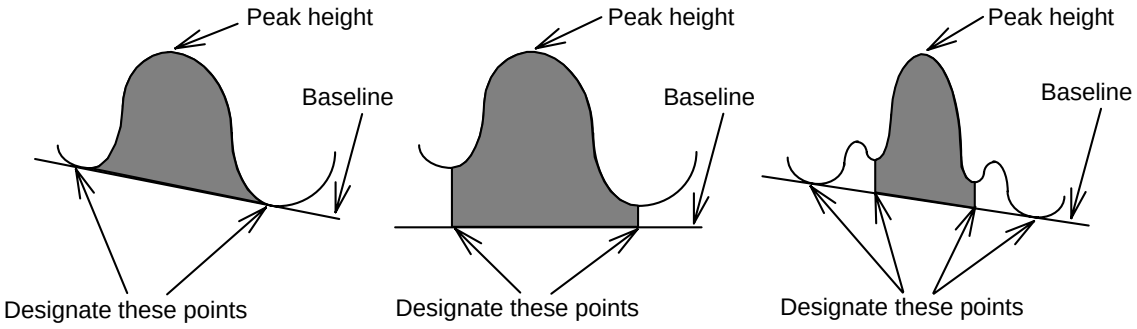


Fig. 2.38 Peak Area detection methods

In addition, three methods are available for calculating the peak area:

(1) Ignore Under Baseline Region
(2) Subtract Under Baseline Region
(3) Add Under Baseline Region

To calculate peak area ①+② in Fig. 2.39, designate a [2 Point Base] from Point A to Point B and select [Add Under Baseline Region]. To calculate peak area ①, designate a [2 Point Base] from Point A to Point B and select [Ignore Under Baseline Region]. To calculate peak area ①-②, designate a [2 Point Base] from Point A to Point B and select [Subtract Under Baseline Region].

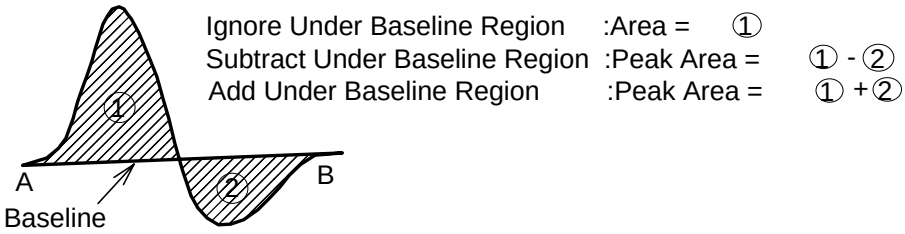


Fig. 2.39 Example 1

Fig. 2.40 Example 2

In Fig. 2.40, when a baseline is designated from point A to B, all three methods give the same result.

The [Peak Area] dialog box contains parameters used to calculate the peak area and the area ratio. Since [Peak Area] dialog box contains many elements, before explaining each element in the dialog box the procedure for calculating peak area is described below.

The following example explains how to calculate peak area using the [2-Point Base] method.

(1) Select [Processing] - [Peak Process] - [Peak Area...] to display the following dialog box.

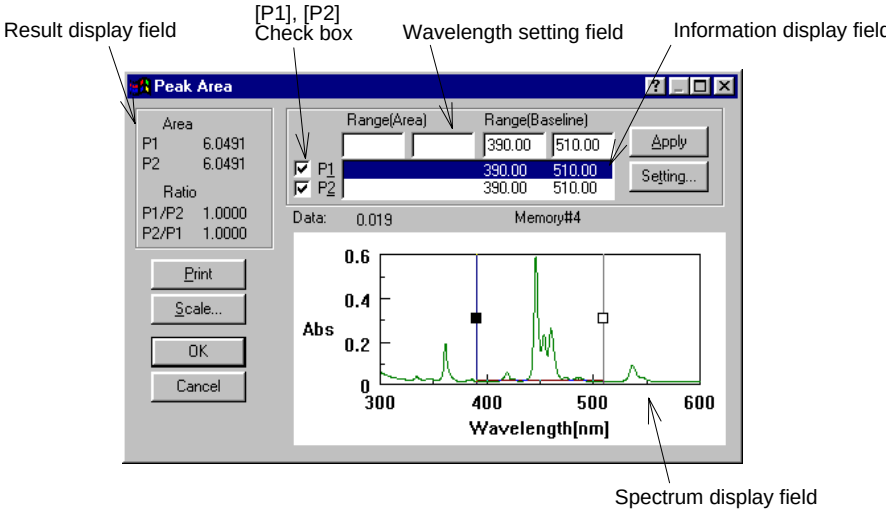


Fig. 2.41 [Peak Area] dialog box

(2) Check the [P1] box to calculate peak area.

Note: [P2] should also be selected when calculating the peak area ratio.

(3) Click <Setting...> to open the [Peak Area - Set] dialog box. Set the peak area calculation method as follows.

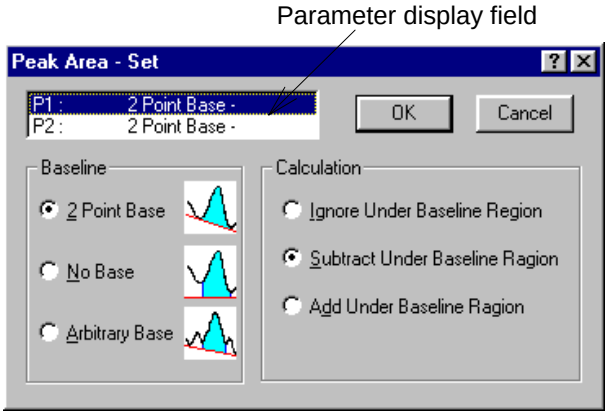


Fig. 2.42 [Peak Area - Set] dialog box

(a) Click on [P1] in the parameter display field to set parameters for [P1].
(b) Select the [2 Point Base] option button in the [Baseline] group.

Note: When calculating peak area ratio, repeat steps 3a) and 3b) replacing [P1] with [P2] to set the parameters for [P2].

(4) Set the base wavelength for Peak 1
(a) Click on [P1] in the information display field. The wavelength at the base position is displayed in [Range(Baseline)] allowing the wavelength to be changed.
(b) Set the base wavelength using the wavelength setting bar on the spectrum. The wavelength can also be set by directly inputting a value into the text box, and then clicking <Apply>. Peak area is calculated and displayed in the results display field.

Note: Set the wavelength for [P2] using the same procedure when calculating peak area ratio.

(5) Click <Print> to open the [Print] dialog box. Click <OK> to print the results.

[Peak Area] dialog box

Results display field:	When the [P1]/[P2] checkboxes are selected, the areas for Peak 1 and Peak 2 are displayed at [P1] and [P2], respectively, and the area ratios of Peak 1/Peak 2 and Peak 2/Peak 1 are displayed at [P1/P2] and [P2/P1], respectively. The results are recalculated and redisplayed each time the wavelengths of the area calculating range and base calculating range are changed.
[P1], [P2]	When these checkboxes are selected, the results are displayed in the results display field.
[Range (Area)], [Range (Baseline)]	These are wavelength ranges for calculating area and drawing the baseline, respectively. Click on and drag the wavelength setting bar to the desired location, or input the values directly. For [2 Point Base], set the wavelength in [Range (Baseline)]. For [No Base], set the wavelength in [Range (Area)]. For [Arbitrary Base], set the wavelength range for drawing the baseline in [Range (Baseline)], and for calculating peak area, set the wavelength in [Range (Area)].
Information display box:	Displays the wavelengths set in [Range (Area)] and [Range (Baseline)] for peak [P1] and [P2] for calculating the peak height/height ratio. Click the wavelength setting box to change the wavelength using the wavelength setting bar.
Spectrum field:	Set the peak and base wavelengths by dragging the wavelength setting bar on the spectrum. The peak area/area ratio is calculated at the same time as it is set. Data from the active wavelength setting bar are displayed at upper-right side of the display beside [Data].
<Apply>	After entering the [Range (Area)] and [range (Baseline)], click <Apply> to move the wavelength setting bar to the designated wavelengths and execute calculation.
<OK>	Closes the dialog box and stores the peak area information in memory.
<Print>	Opens the [Print] dialog box. For details refer to Section 2.1.7.
<Setting...>	Opens the [Peak Area - Set] dialog box.

[Peak Area - Set] dialog box

Parameter display field:	Displays the [P1] and [P2] calculation parameters. Click on [P1] to set the parameters for [P1]. Similarly, for [P2].
[Baseline] group	Contains the available baseline drawing methods.

[2 Point base] Designates two points to determine the area within the baseline range.

[No Base] Designates two points to calculate the area from the zero line.

[Arbitrary Base] Calculates area by designating the wavelength ranges for drawing the baseline and for area calculation separately.

[Calculation] group Select area calculation method from the following three methods. (Refer to Fig. 2.39 and Fig. 40)

[Ignore Under Baseline Region]
[Subtract Under Baseline Region]
[Add Under baseline Region]

<OK> Closes the dialog box and returns to the [Peak Area] dialog box.

2.4.3.4 [Peak Width...]

Select [Processing] - [Peak Process] - [Peak Width...] to display the [FWHM] dialog box used to calculate the full width at half maximum.

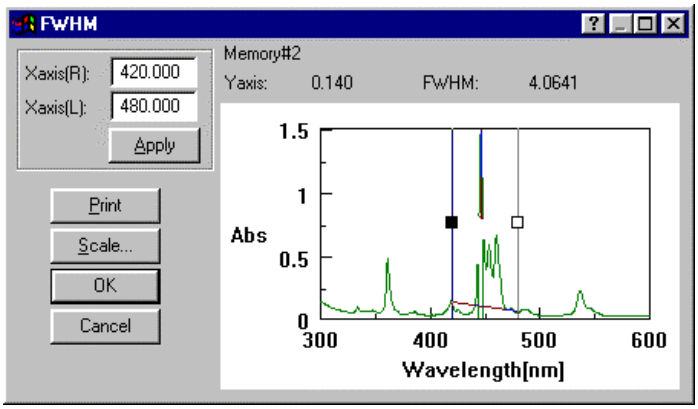


Fig. 2.43 [FWHM] dialog box

Spectrum area: Set the full width at half maximum calculating range by dragging the wavelength setting bar on the spectrum. The full width at half maximum value is calculated simultaneously.

In addition to the wavelength setting bar, the full width at half maximum calculation range can be entered directly in [Xaxis(R)] and [Xaxis(L)].

[Xaxis(R)] Enter the lower X-axis value for the full width at half maximum calculation range.

[Xaxis(L)] Enter the upper X-axis value for the full width at half maximum calculation range.

[FWHM] Displays the result of the full width at half maximum calculation.

<Print> Opens the [Print] dialog box. For details refer to Section 2.1.7.

2.4.4 [Subtraction...]

Select [Processing] - [Subtraction...] to determine a difference spectrum.
One method of identifying an unknown sample is to compare the spectrum of the sample with other known spectra. To identify the components of an unknown mixture, the spectrum of the known components can be removed, leaving only the spectrum of the unknown components of the mixture. Thus, if the spectrum of the mixture is assumed to be A, and the spectrum of known components is assumed to be B, the difference spectrum can be determined using the formula (A × coefficient - B) or the formula (A - B × coefficient). The coefficient should be set to cancel the intensity of a common absorption peak (key band).
The coefficient can be applied using one of two methods. The first method involves continuously changing the coefficient to remove the key band by trial and error while viewing the spectrum. The second method involves calculating a coefficient from an observed peak height or area in order to remove the key band.
The number of spectra overlaid in the view determines which dialog box opens first when [Subtraction...] is executed.

- When one spectrum is displayed, the file [Open] dialog box appears. Select a spectrum to be used for subtraction.
- When two spectra are displayed, the [Subtraction] dialog box appears.
- When three or more spectra are displayed, the [Select Spectrum] dialog box appears. Select a spectrum to be used for subtraction.

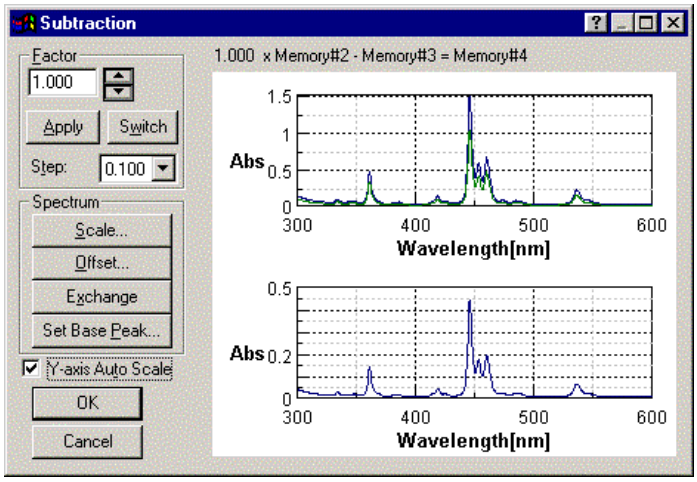


Fig. 2.44 [Subtraction] dialog box

In Fig. 2.44, the resulting difference spectrum of Coefficient × Memory#2 - Memory#4 appears in the lower half of the spectrum display area.

[Factor]	Input a factor. The factor can also be changed using the arrow keys. Each click on an arrow key increases or decreases the factor by the amount designated in [Step]. The difference spectrum is recalculated each time the factor is changed.
[Step]	Designates the increment or decrement by which [Factor] increases or decreases each time an arrow key is clicked.
<Switch>	Exchanges the spectrum to be multiplied by the factor. In the above figure, clicking <Switch> will change the

calculation from Factor × Memory#2 – Memory#4 to Memory#2 – Factor × Memory#4.

Spectrum display area — The spectra are displayed at the top and the difference spectrum below.

[Spectrum] group

<Scale...> — Click to set the spectrum range.

<Offset...> — Click to open the [Subtraction (Offset)] dialog box used to calculate the entire spectrum based on the assumption that the difference between two spectra on a designated horizontal axis is zero.

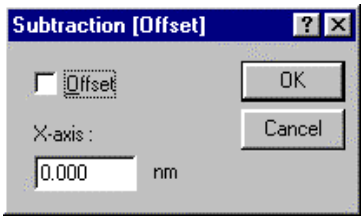


Fig. 2.45 [Subtraction [Offset]] dialog box

When the offset box is checked, calculation is performed based on the assumption that the difference at the horizontal axis designated in [X-axis] is zero.

<Exchange> — Click to exchange spectra. In Fig. 2.44, clicking <Exhange> will change the calculation from Factor × Memory#2 – Memory#4 to Factor × Memory#4 - Memory#2.

<Set Base Peak...> — Click to display the [Subtraction (Set Base Peak)] dialog box used to calculate the factors that offset a particular peak. These factors can be calculated for peak height or area. (The contents of the [Subtraction [Set Base Peak]] dialog box are described below.)

[Y-axis Auto Scale] — Check this box to view the results using the auto scale function. Deselect when viewing the change in the size of the differential spectrum.

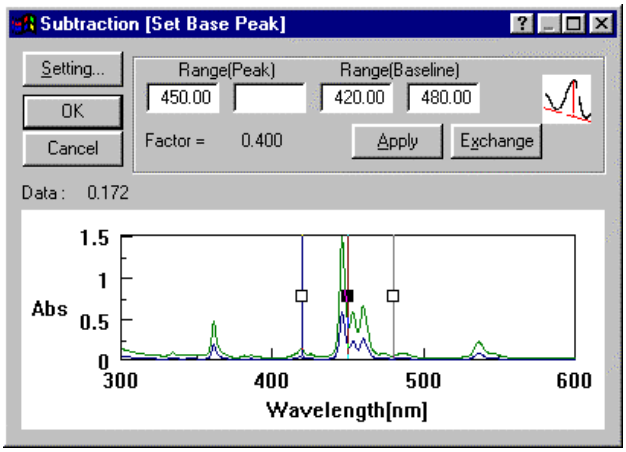
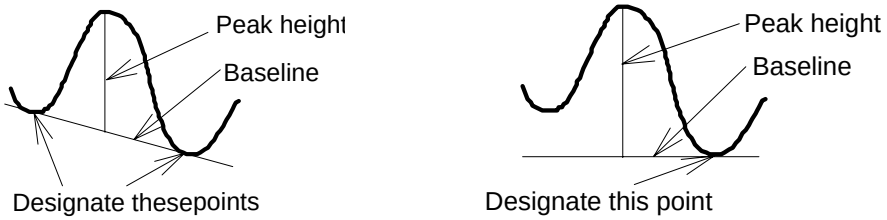


Fig. 2.46 [Subtraction [Set Base Peak]] dialog box

Subtraction [Set Base Peak] dialog box

<Setting...> When determining the factor using the peak height, the following two baseline drawing methods are available.

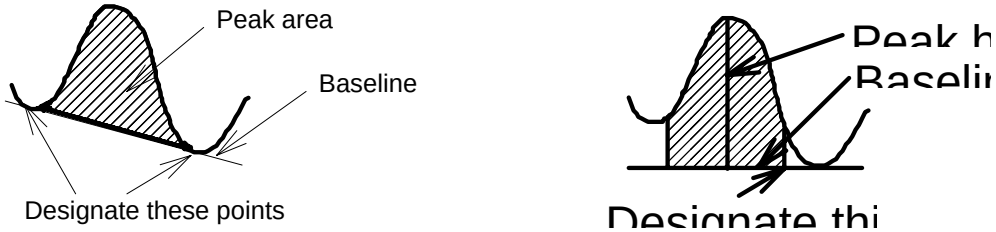


(1) 2-Point base: Designate 2 points to determine the baseline

(2) 1-Point base: Designate 1 point to determine the baseline

Fig. 2.47 Baseline drawing methods when determining factor using peak height

When determining the factor using the peak area, the following two methods are available.



(3) 2-Point base: Determines the zero-level by designating the range.

(4) No base: Calculates area from area within baseline.

Fig. 2.48 Baseline drawing methods when determining factor using peak area

To designate the appropriate method, click <Setting...> and change the parameters in the [Set peak Parameters] dialog box displayed.

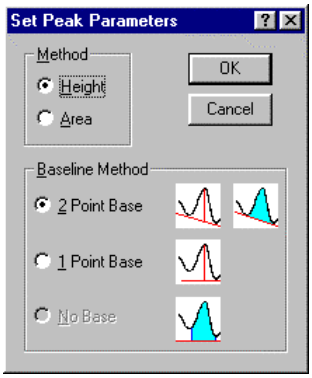


Fig. 2.49 [Set Peak Parameters] dialog box

[Range (Peak)] Wavelength or wavelength range for calculating peak height or area. Click on and drag the wavelength setting bar to the desired location, or input the values directly.
For method (1), input peak wavelength.
For method (4), input area calculating range.

[Range (Baseline)]	Wavelength range for drawing baseline. For methods (1) and (4), input the range of the baseline.
<Apply>	Calculates the factor at the designated horizontal axis value. (When the horizontal axis value is set using the wavelength setting bar, calculation is performed automatically and clicking on <Apply> is not necessary.)
[Data]	Displays the data of the active spectrum at the position of the moving wavelength setting bar. (The spectrum displayed in the small box to the right of <Exchange> is the active spectrum.)
<Exchange>	Click to change the active spectrum. Each click on this button changes the spectrum displayed at right.

2.4.5 [X Unit Conversion...]

Select [Processing] - [X Unit Conversion...] to display the [X-axis Conversion] dialog box used to convert the X-axis units of the spectrum.

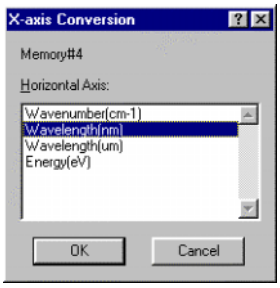


Fig. 2.50 [X-axis Conversion] dialog box

2.4.6 [Y Unit Conversion...]

Select [Processing] - [Y Unit Conversion...] to display the [Y Unit Conversion] dialog box used to convert the Y-axis units of the spectrum.
This function is applicable for spectra for which the vertical axis is absorbance(Abs), %T or %R.

Note: When a spectrum is selected for which the vertical axis is intensity a [Data mode error] message will appear.

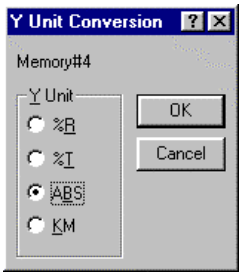


Fig. 2.51 [Y Unit Conversion] dialog box

2.4.7 [Other...]

2.4.7.1 [Comment...]

Select [Processing] - [Other...] - [Comment...] to display the [Comment Edit] dialog box used to add or edit comments.

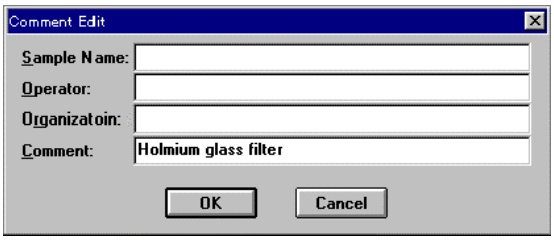


Fig 2.52 [Comment Edit] dialog box

[Sample Name], [Operator], [Organization], and [Comment] can be added or edited. The maximum number of characters that can be input is 62, 62, 62 and 124, respectively.

2.4.8 [Common Option]

2.4.8.1 [Kinetics...]

This function is used with time course data and calculates the enzyme activity value.

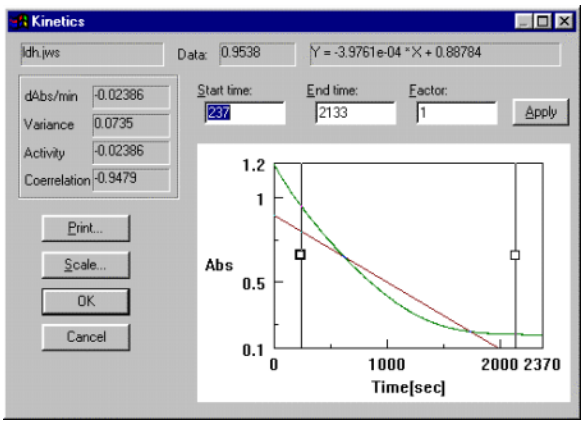


Fig 2.53 [Kinetics] dialog box

Note:	*Immediately after the [Kinetics] dialog box opens, the calculation range is set to the entire region to calculate the result.*

Data display field	Displays time course (reaction curve) data and the range specified with the time setting bar (from calculation start time to calculation end time) approximated with a first-order regression straight line using the least squares method. Set the calculation start time and calculation end time by dragging the time setting bar with the mouse while watching data. The data value of the time setting bar position is displayed in the [Data] field on the data display.
[Start time]	Enter the calculation start time.

[End time]	Enter the calculation end time.
[Factor]	Enter a factor for the kinetics calculation. This value is inherent to the sample.
<Apply>	Click to execute kinetics calculation.
<Print…>	Click to display the [Print] dialog box. In the [Print] dialog box, click <OK> to print the result.

2.4.8.2 [Data Dump...]

Select [Processing] – [Data Dump…] to display the [Data Dump Parameter] dialog box used to view measured data values. This function also allows data values to be copied to the clipboard.

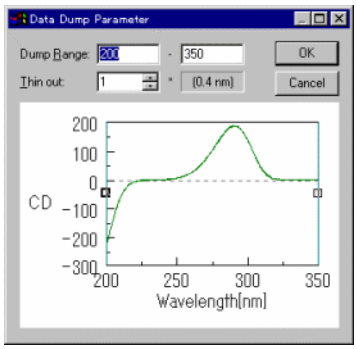


Fig. 2.54 [Data Dump Parameter] dialog box

[Dump Range:]	Specify the range from which to dump data values.
[Thin out:]	Enter the number of points to be thinned out.
<OK>	Click to display the data values in the following dialog box.

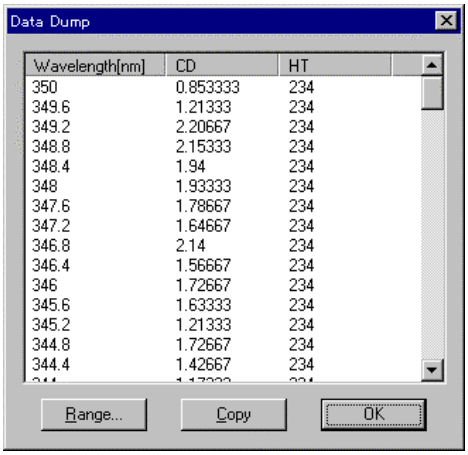


Fig. 2.55 [Data Dump] dialog box

<Range...>	Returns to the [Data Dump Parameter] dialog box.
<Copy>	Copies data to the clipboard.
<OK>	Closes the dialog box.

2.4.8.3 [Move Channel...]

Select [Processing] - [CD Options] – [Move Channel …] to display the [Channel Conversion] dialog box used to move channels (for example, channel 1 and channel

2) in a view or pick up only data of a desired channel from data overlaid in a view or from multiple-channel data.
This function is used in the following cases.
(1) To process the data of, for example, channels 2 to 4. That is, these data must be moved to channel 1.
(2) To pick up only the data of a desired channel and display it in a new view.

Note: Only channel 1 data can be processed.

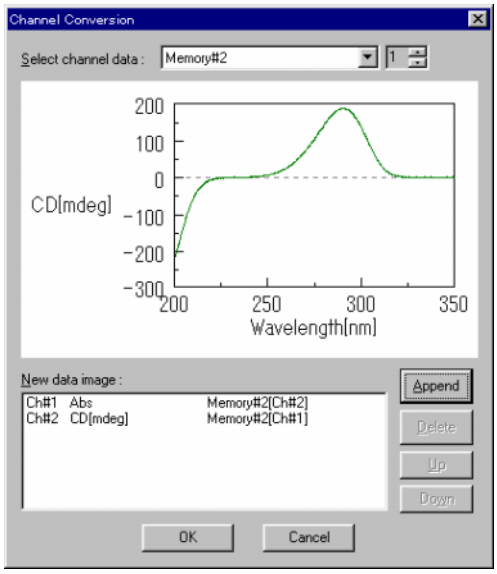


Fig. 2.56 [Channel Conversion] dialog box

[Select channel data:] Select the filename of the desired data from the filename drop-down list and then designate a channel by clicking on the up and down arrow buttons ([▲] [▼]) at right. The data shown in the spectrum display area are rewritten with the designated data.
When the desired data are displayed, click the <Append> button. The designated data are registered in [New data image:]. Data registered first are entered in channel 1. Repeat this step to move channels. To pick up desired data only, register only the required data.

Note: The filename can be selected when multiple data are overlaid.

[New data image:] Displays designated data register field(s). Maximum of four channels, 1 to 4, from top to bottom.

<Append> Registers the current selection (displayed in the spectrum display field) in the [New data image:] list.

<Delete> Deletes the currently selected item in [New data image:].

<Up> Moves the currently selected item up the [New data image] list. Used to change the registered data display channel.

<Down> Moves the currently selected item down the [New data image] list. Used to change the registered data display channel.

<OK> Click to close the dialog box and open the registered data in a

new view.

2.4.8.4 [Arithmetic with Data...]

Performs arithmetic operation using data overlaid in the same channel of a view. However, the arithmetic operation cannot be performed unless the data mode and data interval of the data of each overlaid channel are the same. The horizontal axis is limited to the range in which the two data sets are overlaid. If only one set of data is displayed, calculation is performed between the data and a constant or constants.
Select [Processing] – [CD Options] – [Arithmetic with Data…] to display the [Arithmetic with Data] dialog box.

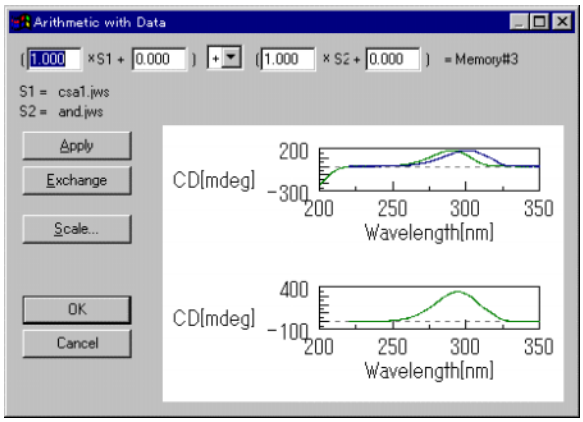


Fig. 2.57 [Arithmetic with Data] dialog box

Calculation is performed according to the expression designated at the top of the dialog box. To construct an arithmetic operation enter numerical values in each text box as desired and select the appropriate operator from the drop-down list.

Spectrum display area	The data before arithmetic operation are displayed at the top and the result of the arithmetic operation is displayed at the bottom.
<Apply>	Click to perform calculation.
<Exchange>	Exchange data S1 and S2 with each other.
<Scale...>	Click to display the [Scale] dialog box used to change the scale of the original data.
<OK>	Click to perform calculation and close the dialog box. The result of arithmetic operation is displayed in a new view.

Note: When using data overlaid in the same channel of a view, to perform calculation between one set of data and a constant or constants enter 0 for the coefficient of the unwanted data set.

Note: If only one set of data is displayed in the view, the dialog box shown in Fig. 2.67 is displayed. Calculation can be performed between the data and a constant or constants.

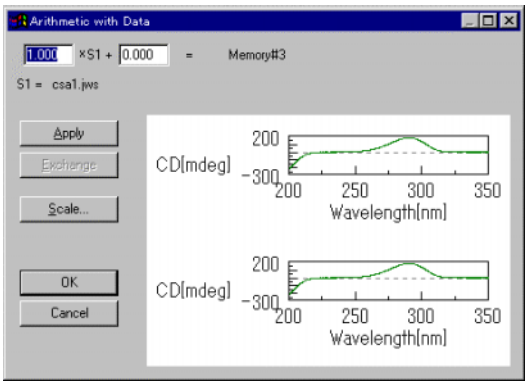


Fig. 2.58 [Arithmetic with Data] dialog box (with one piece of data)

2.4.8.5 [Arithmetic with Channel...]

This function performs arithmetic operation using data displayed in the same view. Unlike the [Arithmetic with Data...] function above that performs arithmetic operation using data overlaid in the same channel, this function performs arithmetic operation using data freely selected from multiple channels of data displayed in a view. Needless to say, overlaid data can also be selected. In addition, the vertical axis attribute can be freely selected. The horizontal axis is limited to the range in which the two sets of data are overlaid.

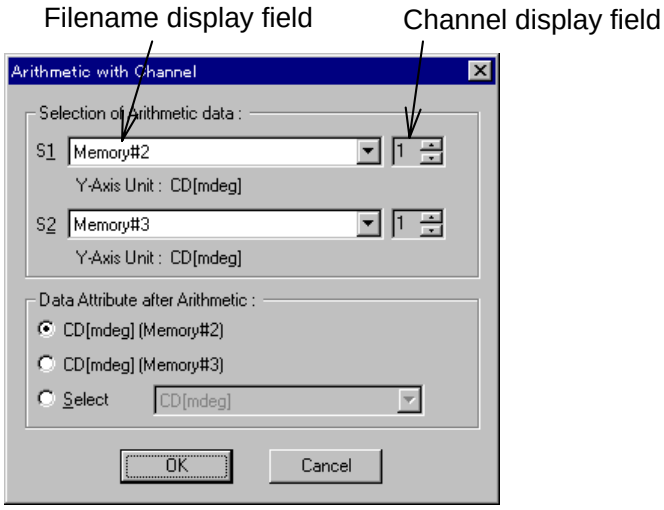


Fig. 2.59 [Arithmetic with channel] dialog box

[Selection of arithmetic data:] group — Select the filenames of the desired data from the [S1] and [S2] drop-down lists and then designate channels by clicking on the up and down arrow buttons ([▲] [▼]) at right. In the example screen above, data overlaid in channel 1 are calculated.

[Data Attribute after arithmetic:] — Select the vertical axis attribute of the data after arithmetic operation.
If the vertical axis attribute changes after arithmetic operation, click the [Select] option button and select the vertical axis attribute from the drop-down list on the right. For example, the result of division by single beam (SB) will be %T.

<OK> — Click to display the following dialog box.

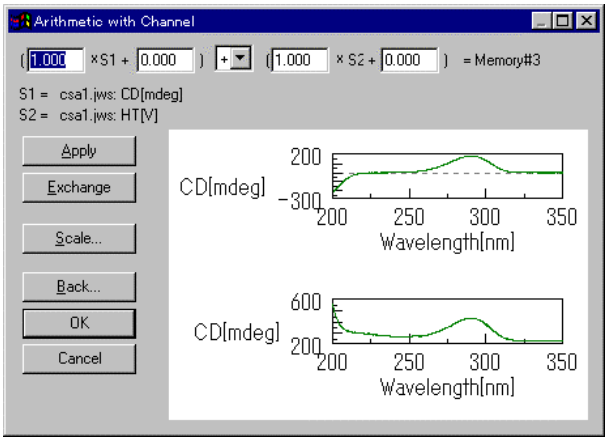


Fig. 2.60 [Arithmetic with Channel] dialog box

Calculation is performed according to the expression designated at the top of the dialog box. To construct an arithmetic operation enter numerical values in each text box as desired and select the appropriate operator from the drop-down list. Refer to Section 2.4.11.5 for more information. Click <Back...> to return to the previous dialog box shown in Fig. 2.66.

2.4.8.6 [Data Accumulation]

Accumulates data overlaid in the same channel of a view and displays the result in a new view.

Note:	*Data cannot be accumulated unless the data mode, data interval and measurement range of each overlaid channel are the same.*

2.4.9 [IR-option]

2.4.9.1 [ATR Conversion…]

This option converts the absorption intensity relationship between the high wavenumber side and low wavenumber side.
This is only effective for specctra measured by the ATR method. Although calculation can be performed for other data, the results are meaningless.

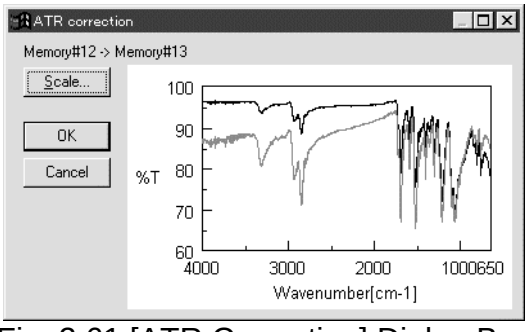


Fig. 2.61 [ATR Correction] Dialog Box

2.4.9.2 [IF to Spectrum…]

This option converts an interferogram(IF) into a single-beam spectrum(Single). Eleven types of apodization functions are available.

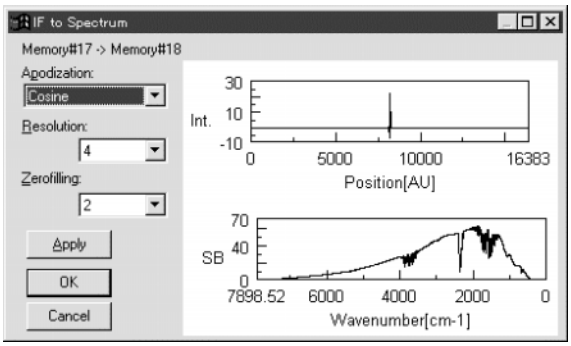


Fig. 2.62 [IF to Spectrum] Dialog Box

Spectrum display area	Display the original spectrum at the top, and the single-beam spectrum below.
[Apodization]	Ste the desired spodization function here.
[Resolution]	Set the spevtrum resolution here. Note that a resolution lower than that of the interferogram cannot be set.
[Zerofilling]	Set whether zero filling is to be done here.
<Apply>	Click this button to perform calculation using the set parameters and display the spectrum.

2.4.9.3 [Spectrum to IF…]

This option converts a single-beam spectrum(Single) into an interferogram(IF). There are no parameters.

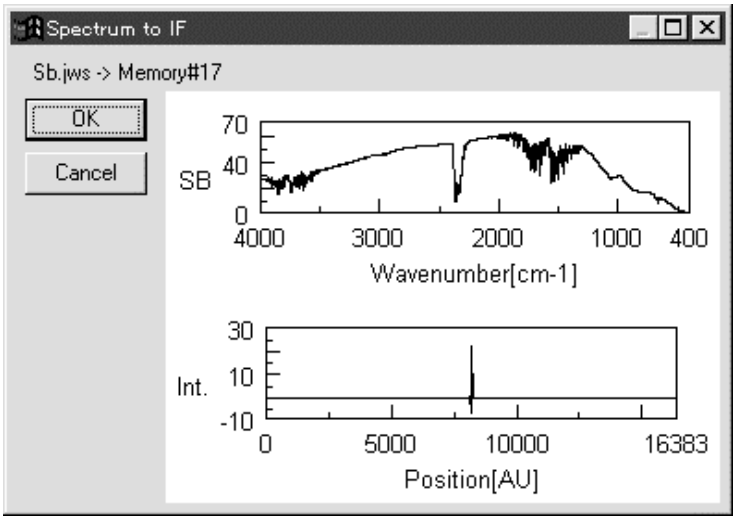


Fig. 2.63 [Spectrum to IF] Dialog Box

Spectrum display area	Display the original spectrum at the top, and the interferogram below.

2.4.10 [FP-option]

2.4.10.1 [Phospho. Lifetime...]

Select [Processing]-[FP Options]-[Phospho. Lifetime...] to display the [Phosporescent Lifetime Analysis] dialog box used to calculate the phosphorescent lifetime.

Note:	*Refer to Section 4.4 of the Appendix for more information on phosphorescent lifetime.*

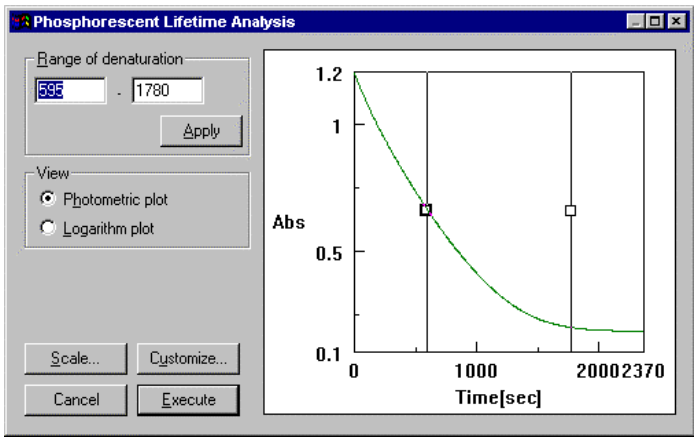


Fig. 2.64 [Phosphorescent Lifetime Analysis] dialog box

[Range of denaturation] Click and drag the time setting bar in the Spectrum display area to the desired location, or input the values directly.

[View] Select the appropriate option button to display the spectrum using either a photometric or logarithmic scale.

<Scale...> Click to display the [Scale] dialog box used to change the display scale of the spectrum.

<Customize...> Click to display the [Customize] dialog box used to designate the printing style.

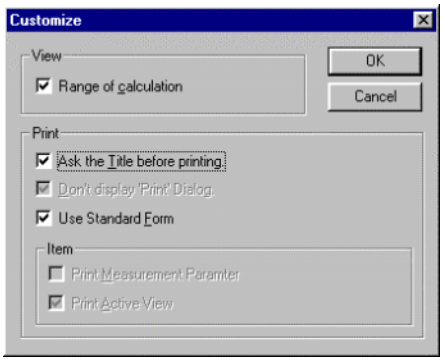


Fig. 2.65 [Customize] dialog box

[Execute] Click to calculate phosphorescent lifetime. The calculated results will be displayed in a dialog box.

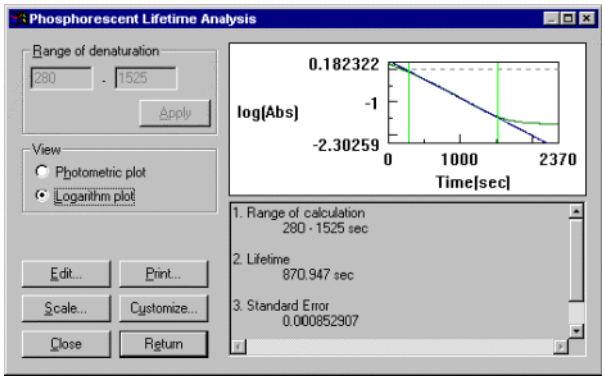


Fig. 2.66 [Phosphorescent Lifetime Analysis] result dialog box

[Phosphorescent Lifetime Analysis] result dialog box

<Edit...> Click to display the [Edit] dialog box used to copy the phosphorescent lifetime analysis results to the clipboard.

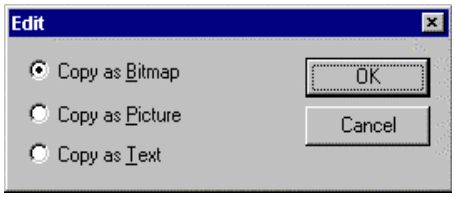


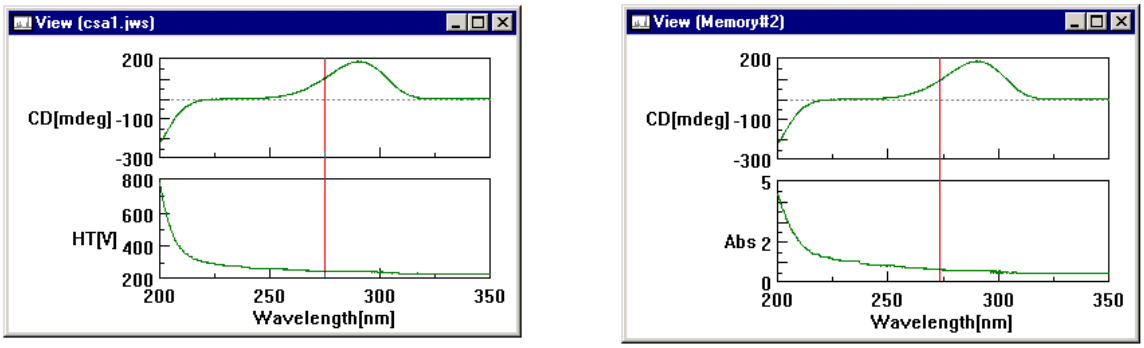
Fig. 2.67 [Edit] dialog box

<Print...> Click to display the [Print] dialog box. For details refer to Section 2.1.7.

2.4.11 CD Options

2.4.11.1 [HT → OD…]

This function converts HT voltage data to absorbance. To convert the currently active view data, select [Processing]-[CD Option]-[HD -> OD...]. The converted data are displayed in a new view.



HT data view (before conversion) Absorbance data view (after conversion)

Fig. 2.68 HT voltage to absorbance conversion

2.4.11.2 [Optical constant calculate...]

This function is used to calculate optical constants. The types of calculation available are shown in Table 1. The dialog box displayed differs depending on whether the

active view contains multiple-channel data or single-channel data. Each dialog box is explained below.

Table 1 Optical constant calculations

Data mode (channel 1)	**Type of calculation**	**Y-axis units of result view**
CD	Molecular ellipticity Specific ellipticity Molecular CD absorption CD absorption	Mol.Ellip., Mol.Ellip.MG Spc.Ellip., Spc.Ellip.MG Mol.CD, Mol.CD MG Delta OD
Mol.Ellip., Mol.Ellip.MG	Molecular CD absorption	Mol.CD, Mol.CD MG
ORD	Molecular rotation Specific rotation	Mol.Rotation, Mol.Rot.MG Spc.Rotation, Spc.Rot.MG
LD		LD Corr. Delta Eps.(LD) Delta E(LD)
%T	Absorbance Specific absorbance Molecular absorbance	Abs Spc.Abs Mol.Abs
Abs	Transmittance Specific absorbance Molecular absorbance	%T Spc.Abs Mol.Abs

1) Dialog box displayed for multiple-channel data

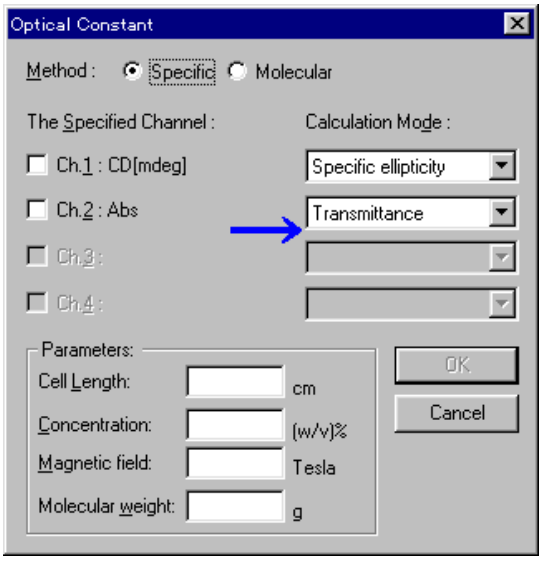


Fig. 2.69 [Optical Constant] dialog box (multiple-channel data)

[Method:]	
[Specific]	Select when calculating specific ellipticity and delta OD.
[Molecular]	Select when calculating molecular ellipticity and molecular circular dichroic absorption.
[The Specified Channel:]	Check the channels to be used for the calculation.
[Calculation Mode:] drop-down list	Select the desired data mode for each selected channel.
[Parameters:] group	Calculation parameters. Enter the parameters required for calculation.
[Cell Length:]	Light path length of cell
[Concentration:]	Sample concentration
[Magnetic field:]	Magnetic field intensity
[Molecular weight:]	Molecular weight
<OK>	Click to perform calculation. The results are displayed in a new view. The units of the vertical axis displayed in the resulting view are shown in Table 1.

2) Dialog box displayed for single-channel data

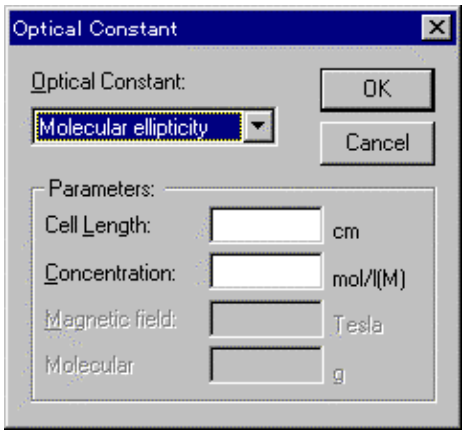


Fig. 2.70 [Optical Constant] dialog box (single-channel data)

[Optical Constant:] drop-down list	Select the desired optical constant calculation (refer to Table 1).
[Parameters:] group	Calculating parameters. Enter the parameters required for calculation. (The active parameters vary with the type of calculation).
[Cell Length:]	Light path length of cell
[Concentration:]	Sample concentration
[Magnetic field:]	Magnetic field intensity
[Molecular weight:]	Molecular weight
<OK>	Click to perform calculation. The results are displayed in a new view. The units of the vertical axis displayed in the resulting view are shown in Table 1.

2.4.11.3 [KK conversion…]

Select [Processing] - [CD Options] – [KK Conversion…] to display the [KK Conversion] dialog box used to convert CD data to ORD or ORD data to CD. Conversion is performed using the following Kronig-Kramers equation.

Molecular rotation: $$[M_K(\lambda)] = \frac{2}{\pi}\int_a^b \frac{[\theta_K(\lambda')]\lambda'}{(\lambda^2 - \lambda'^2)} d\lambda'$$

Molecular ellipticity: $$[\theta_K(\lambda)] = \frac{2}{\pi\lambda}\int_a^b \frac{[M_K(\lambda')]\lambda'^2}{(\lambda^2 - \lambda'^2)} d\lambda'$$

Here, K denotes the k^{th} electron transition. The integrated wavelength range (from a to b) of CD gives a wavelength which can be regarded as a baseline sufficiently far from the wavelength region of the k^{th} CD band. Therefore, the CD or ORD spectrum obtained by this equation shows partial contribution from a number of electron transitions ranging from the near-infrared to the vacuum ultraviolet region. For example, an ORD spectrum converted from a CD spectrum in the visible to ultraviolet region does not contain any contribution from electron transitions in the far ultraviolet

to vacuum ultraviolet region. It should be noted that for this reason, the converted ORD spectrum and the actually measured ORD spectrum do in agree. Direct numerical integration is performed for calculation, however, the method proposed by Emeis et al. (C. A. Emis et al., Proc. Roy. Soc. (London), A297, 54-65, 1967) is used at singular points.

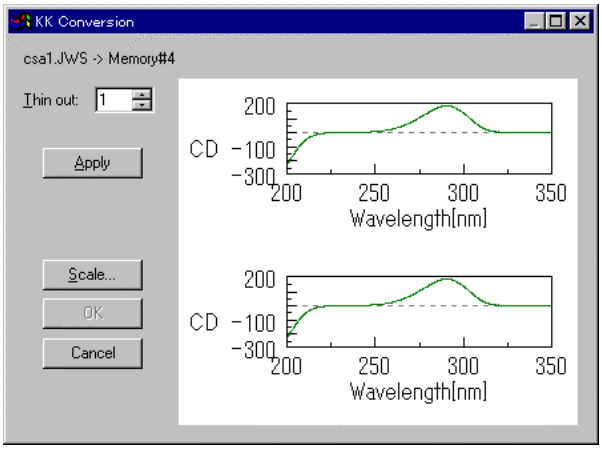
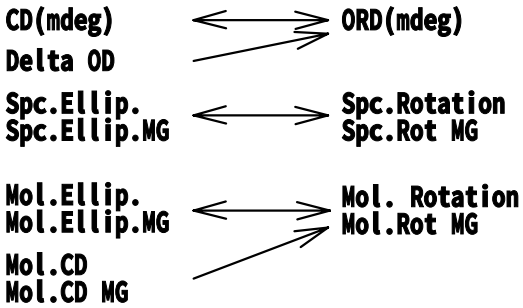


Fig. 2.71 [KK Conversion] dialog box

Spectrum display area	Before conversion, both the top and bottom spectra display the original spectrum. After conversion, the bottom spectrum displays the converted spectrum.
[Thin out:]	Designate the number points to be thinned out.
<Apply>	Click to execute KK conversion.
<Scale...>	Click to display the [Scale] dialog box used to change the scale of the original spectrum.
<OK>	Click to close the dialog box and display the result in a new view.

Photometric modes that permit KK conversion

The following photometric modes permit KK conversion.



Cautions in K/K conversion (CD to ORD conversion)

- The ORD spectrum after conversion will be distorted if either of the wavelength end from the CD spectrum is not zero.
- Perform measurement so that the number of data points of one CD band is 50 or more when the CD spectrum is regarded as a Gaussian curve (C. A. Emis et al. Proc. Roy. Soc. (London), A297, 54-65, 1967).
- The ORD spectrum obtained by conversion and the measured ORD spectrum do not agree. Since the ORD spectrum obtained by conversion is the

contribution from only the wavelength region of the CD spectrum before conversion, the ORD spectrum obtained by subtracting the ORD spectrum obtained by conversion from the measured ORD spectrum represents the contribution from outside the wavelength region of the CD spectrum before conversion. This principle may be applied to estimate the Cotton effect of a wavelength region that cannot be measured.

Cautions in K/K conversion (ORD to CD conversion)

- The wavelength range of ORD that contributes to one CD band ranges from infinitesimal to infinity. Therefore, the ORD spectra that can be measured are within a limited wavelength range because of instrumental limitations. Therefore, the CD spectra after conversion are generally distorted.
- When only one Cotton effect exists and it is near the center of the measurement wavelength range, the distortion of the CD spectrum after conversion is relatively small. In practice, however, it is often the case that multiple Cotton effects exist overlapped in a short wavelength region. In such a case, the CD spectrum after conversion is distorted greatly.

2.4.11.4 [G Value...]

$\Delta\varepsilon$ divided by ε is called G value. It is generally expressed by the following equation.

$$G = \frac{\Delta\varepsilon}{\varepsilon} = \frac{\Delta Abs}{Abs}$$

The G value represents the degree of asymmetry of the absorption band. It can be used as an index of the asymmetric yield of asymmetric synthesis.
The equation for calculating the G value in each data mode is given below.

G=CD(mdeg)/(32980∗Abs)
G=ΔOD/Abs
G=Spc.Ellip/(32980∗Spc.Abs)
G=Mol.Ellip/(3298∗Mol.Abs)
G=Mol.CD/Mol.Abs

Note: Display the data required for calculation in the same view.

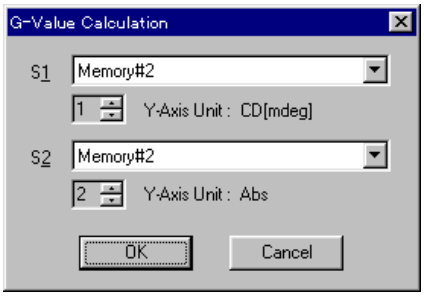


Fig. 2.72 [G-Value Calculation] dialog box

[S1:] Designate the data that will be the numerator in the G value calculation. First, select the filename of the desired data from the drop-down list and then designate the data channel with the up and down arrow buttons ([▲] [▼]).

[S2:] Designate the data that will be the denominator in the G value calculation. The method of designating data is the same as

[S1].

<OK> Click to perform the calculation. The dialog box closes and the calculated data are displayed in a new view.

2.4.11.5 [pH Conversion]

Note:	*This function is only available when the optional [Automatic Titration Measurement] program is installed.*

When this function is executed, a new view is opened and CD value (or fluorescence, HT or other) is displayed on the vertical axis and pH data on the horizontal axis (see Fig. 2.73).

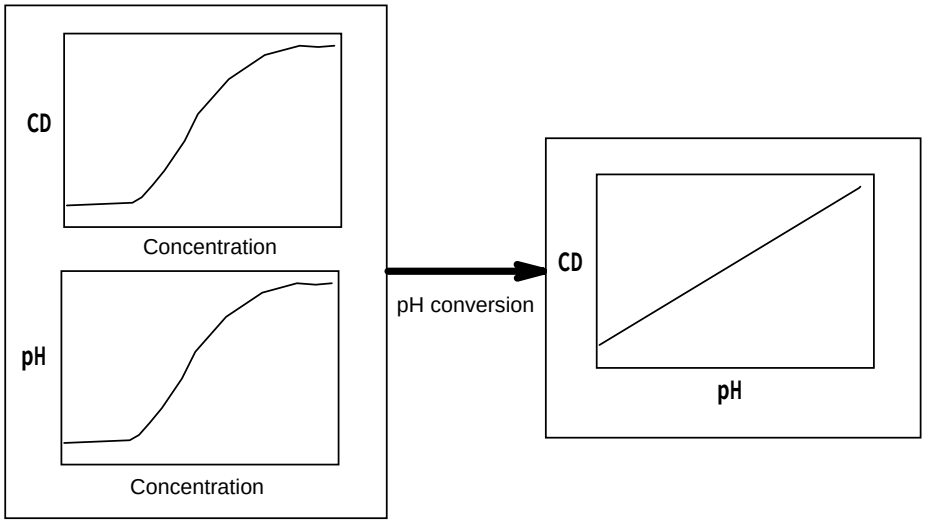


Fig. 2.73 pH conversion (example)

2.5 [Window] Menu

The commands contained in the [Help] menu are described below.

[Cascade]	Cascades all open views.
[Tile]	Tiles all open views.
[Arrange Icons]	Arranges minimized window icons.
[Close All]	Closes all views. If the spectrum data has been changed or if the data is new, a message is displayed which asks if you wish to save before closing. Click [Yes] to save the data before closing. Click [No] to close the view without saving. Click [Cancel] to cancel closing the view.

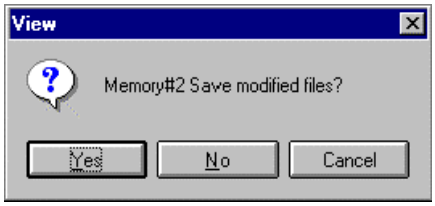


Fig. 2.74 Save message

2.6 [Other] Menu

This section describes the commands contained in the [Other] menu.

[Tool Bar...]	Displays the [Edit Tool Bar] dialog box used to add or remove tool bar buttons.
[Customize...]	Displays the [Customize] dialog box used to change the view and print style options.
[Format...]	Displays the [Format Setting] dialog used to set the number of decimal places used for the X and Y axes. The settings are applied to peak detection results and the X and Y axes values shown in the status bar.

2.6.1 [Tool Bar]

Select [Other] - [Tool Bar…] to display the [Edit Tool Bar] dialog box used to add or remove buttons to or from the tool bar. Of the buttons on the tool bar, there are 11 standard buttons that cannot be changed.

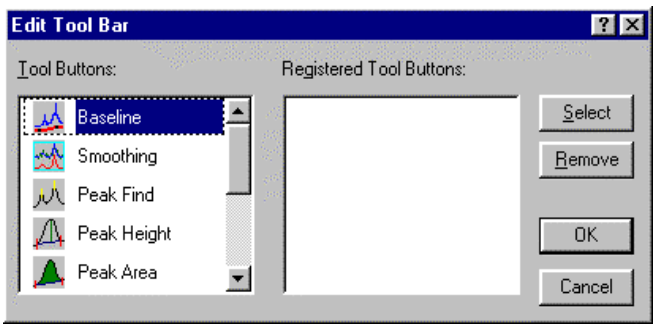


Fig. 2.75 [Edit Tool Bar] dialog box

[Tool Buttons]	Lists the available tool bar buttons. Select buttons to be registered from this list.

[Registered Tool Buttons]	Lists the currently registered tool bar buttons. Select buttons to be deleted from this list.
<Select>	Click to add the currently selected button(s) in the [Tool Buttons] list to the [Registered Tool Buttons] list.
<Remove>	Click to remove the currently selected button(s) in the [Registered Tool Buttons] list from the [Tool Buttons] list.
<OK>	Click to apply the current settings and close the dialog box.

2.6.2 [Customize...]

Select [Other] - [Customize] to display the [Customize] dialog box used to change the view and print style options.

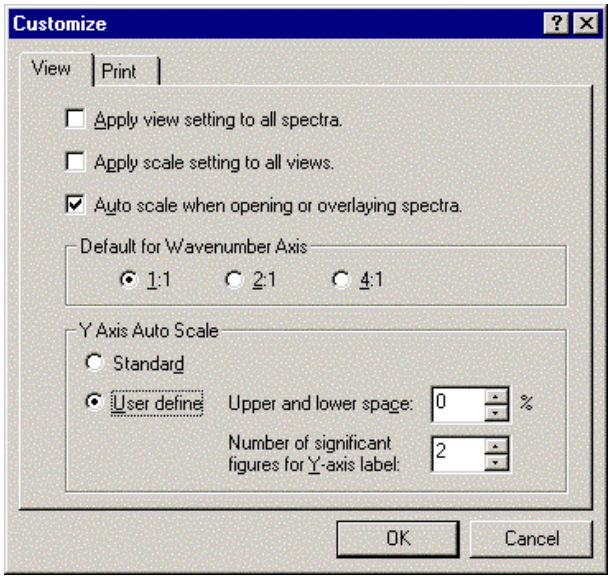


Fig.2.76 [Customize] dialog box showing the [View] tab

[View] Tab

[Apply view setting to all spectra]	Check this box to apply the parameter settings of [Pattern], [Font], and [Grid] in the [View] menu to all views.
[Apply scale setting to all views]	Check this box to apply the parameter settings of [Scale] in the [View] menu to all views.
[Auto Scale when opening or overlaying spectra]	Check this box to use the auto scale function for the Y-axis when opening or overlaying spectra.
[Default for Wavenumber Axis] group	Select the default setting for the Wavenumber axis. Select: 1:1 for an equal interval scale 2:1 for a 1/2 scale on and after 2000 cm-1 4:1 for a 1/4 scale on and after 2000 cm-1
[Y Axis Auto Scale] group	Allows customization of the settings used for the Y-axis auto scale.
Standard	Fits the Y-axis scale to the maximum and minimum values displayed in the View.

User define

Upper and Lower	Automatically calculates the Y-axis scale with a specified proportion of blank space above and below the maximum and minimum values displayed in the View. Setting range from 0 to 20%.
No. of significant figures for Y axis label	Specifies the number of significant figures to be used for the Y-axis label. Setting range from 2 to 6 significant figures. The Y-axis label is always rounded up.

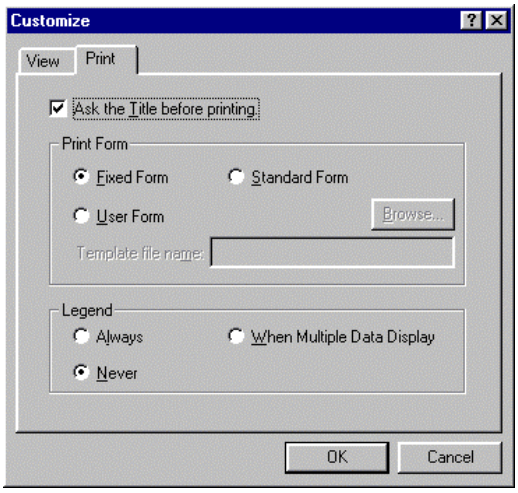


Fig. 2.77 [Customize] dialog box showing the [Print] tab

[Print] Tab

[Ask the Title before printing]	Check this box to be prompted for a title before printing.
[Print Form] group	
[Fixed Form]	Select to print using standard format
[Standard Form]	Select to print using the standard format.
[User Form]	Select to print using a template file created in JASCO Canvas. Click the [Browse] button and designate the JASCO Canvas template file to be used.
[Legend] group	
[Always]	Select to always print a legend with spectra.
[Never]	Select to never print a legend with spectra.
[When Multiple Data Displayed]	Select to print a legend with spectra only when multiple data are displayed.

2.6.3 [Format...]

Select [Other] – [Format…] to display the [Format Setting] dialog box used to set the number of decimal places used for the X and Y axes. The settings are applied to peak detection results and the X and Y axes values shown in the status bar.

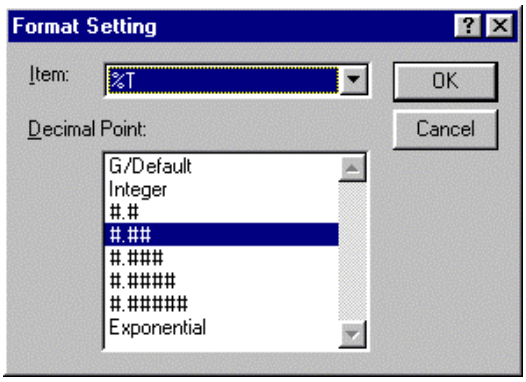


Fig. 2.78 [Format Setting] dialog box

[Item]	Select the units to be set from the drop-down list.
[Decimal Point]	Select the desired format to be applied to the units selected in [Item].

2.7 [Help] Menu

The commands contained in the [Help] menu are described below.

[Contents]	Displays the help table of contents.
[Search topic]	Displays help by keyword.
[About...]	Displays a dialog box containing version information for the Spectra Analysis Program.

3 File Find Program

The File Find program is used to search for previously saved JASCO spectrum files. This section describes how to use the program and contains reference information.

3.1 File Find Method

Use the following procedure to search for previously saved spectra.

(1) Double-click [File Find] in the [Analysis] pane of the [Spectra Manager] window to start the File Find program. The [File Find] window opens. The program can also be started by selecting [File] - [Find…] in the [Spectra Analysis] program.

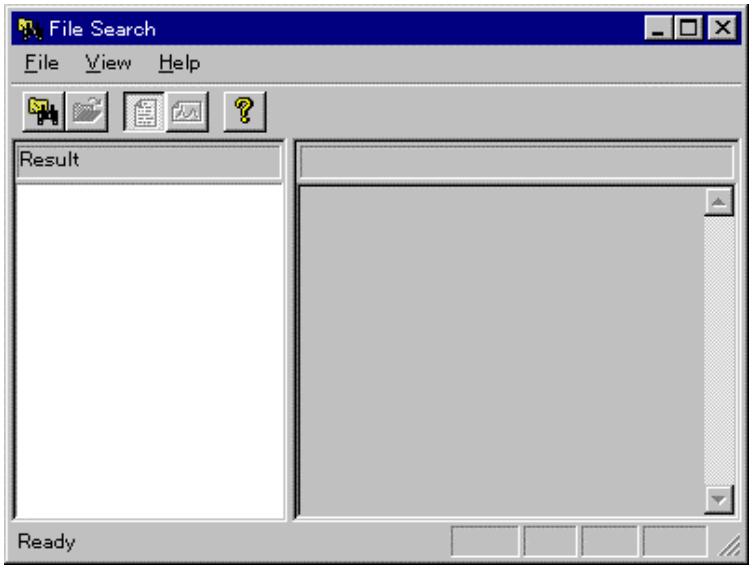


Fig 3.1 [File Find] window

(2) Click the  button to display the [Search Condition] dialog box.

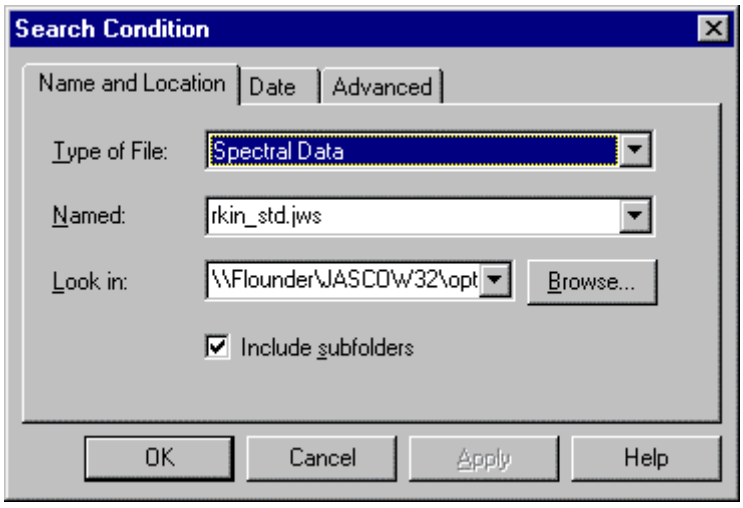


Fig. 3.2 [Search Condition] dialog box

Select the file type, filename (wildcard characters may be used), and where to look for the file (directory and drive).

Note:	*When [Include subfolders] is selected, the program also searches in all the subdirectories beneath the directory selected in [Look in;].*

(3) Click the<OK>button to begin searching. The search results are displayed in the filename display area (Fig. 3.3).

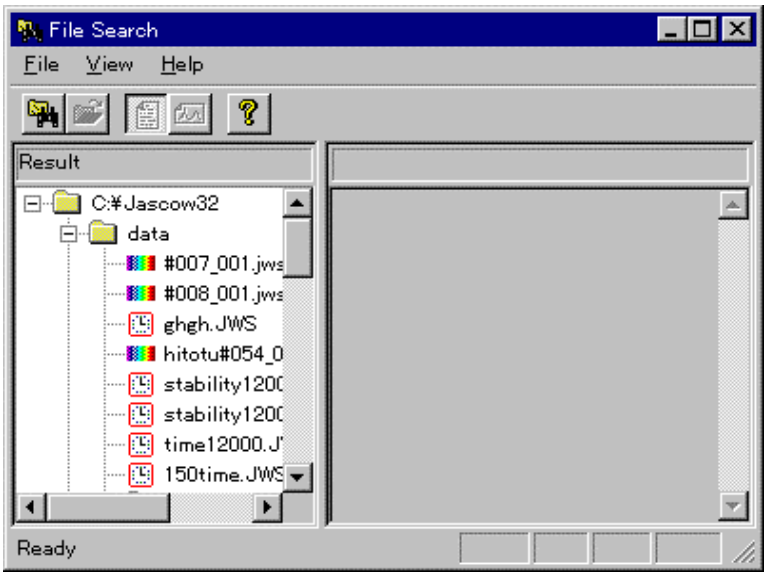


Fig. 3.3 [File Find] dialog box showing search results (when file is not selected)

(4) Click the desired data file in the filename display area. A preview of the spectrum or data information contained in the file is displayed as shown in Fig.3.4 and Fig.3.5.

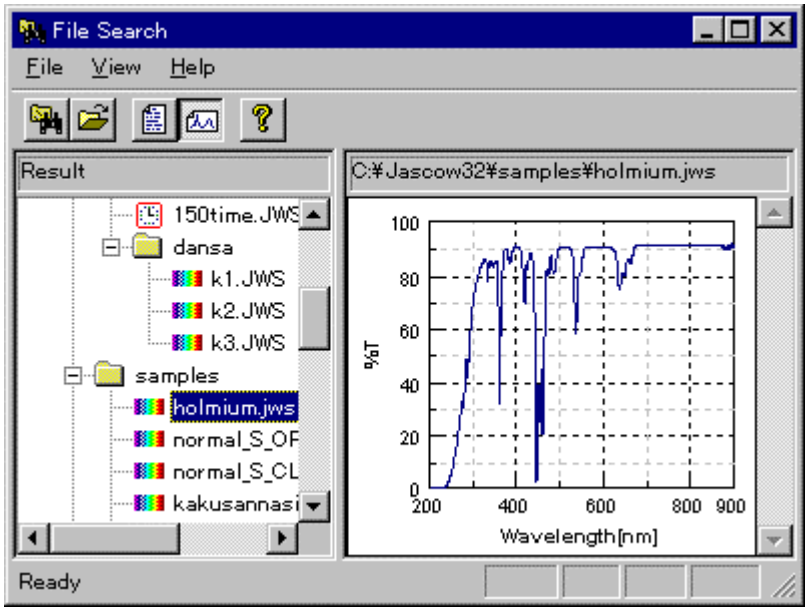


Fig. 3.4 [File Find] dialog box (spectrum preview)

Note:	*In Fig.3.4, a spectrum is displayed in the spectrum/data information display area. When [Information] is selected using the*  *button, the spectrum is rewritten with data information.*

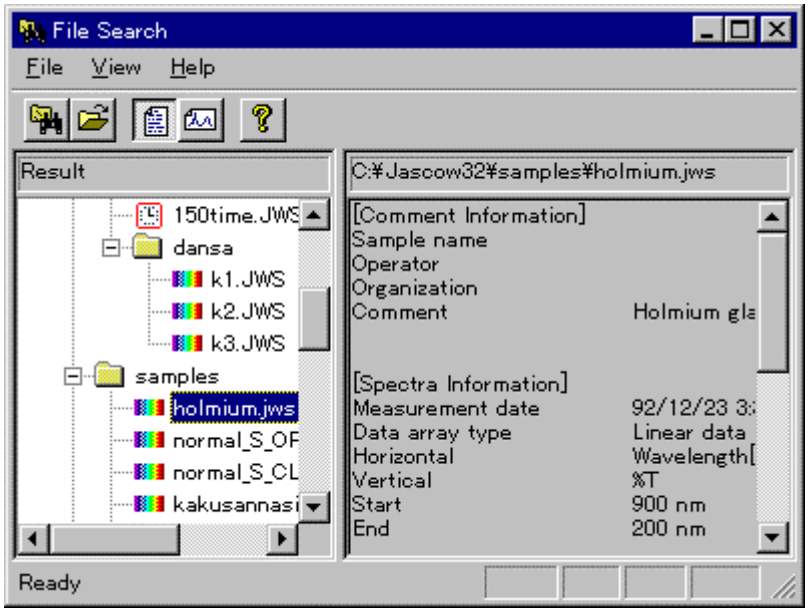


Fig. 3.5 [File Viewer] dialog box (data information)

(5) Finally, click the  button to open the currently selected file. The [Spectra Analysis] program starts, as shown in Fig. 3.6 and a new view opens, displaying the specified spectrum.

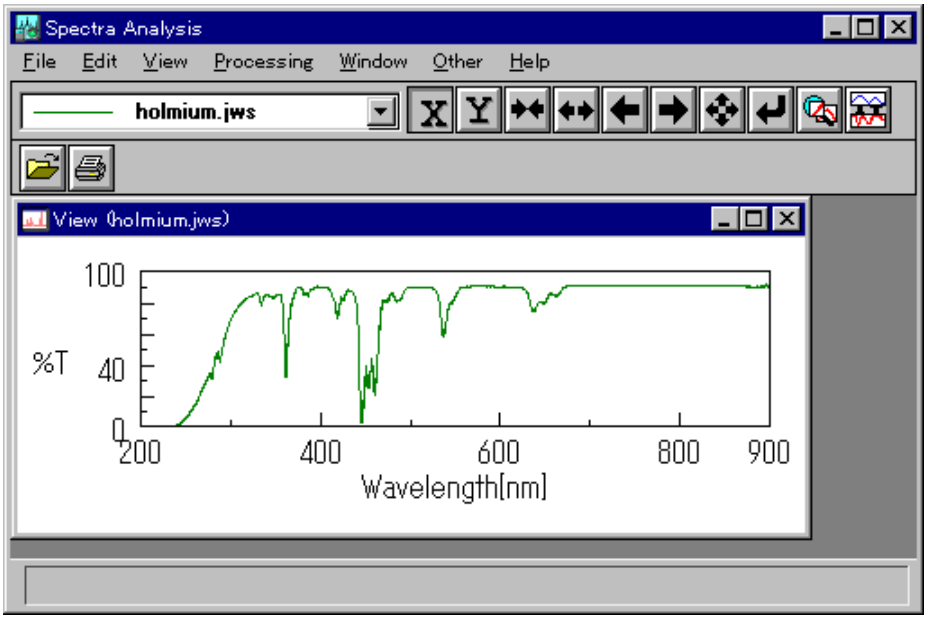


Fig. 3.6 [Spectra Analysis] window

3.2 File Find Program Reference

This section contains reference information for the File Find program.

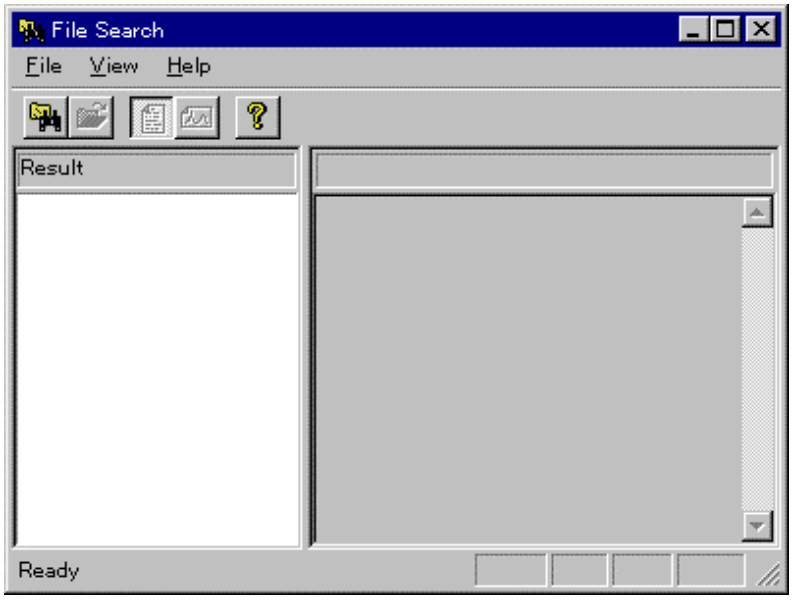


Fig. 3.7 [File Find] dialog box

Note: When the [File Viewer] program is started, nothing is initially displayed in the [File Find] dialog box.

Filename display area	Displays the results of a file search. Spectrum data files indicated by vertically-striped icons, and time course data are indicated by clock icons.
Spectrum/data information display area	Displays a preview of the contents of the currently selected file. Two types of preview are available: spectrum and data information (measurement parameters, etc.).

File menu

[Search] or 	Opens the [Search Condition] dialog box used to specify search parameters and execute a search. Refer to Section 3.2.1 for more information.
[Open] or 	Opens the currently selected data file in the filename display area. If not already running, the [Spectra Analysis] program starts and the file is displayed in a new view (see Fig. 3.6).
[Exit]	Exits the program.

View menu

[Toolbar]	Check to display the tool bar.
[Status Bar]	Check to display the [Status Bar] (at the bottom of [File Find] dialog box).
[Graph] or 	Select to display a spectrum preview in the spectrum/data information display area. Active when a file is selected in the filename display area.
[Information] or 	Select to display spectrum information such as,

measurement parameters, etc. in the spectrum/data information display area. Active when a file is selected in the filename display area.

Help menu

[Help Topics...]	Display help table of contents.
[Search topic]	Allows you to search the help topics.
[About]	Displays version information for the [File Find] program.

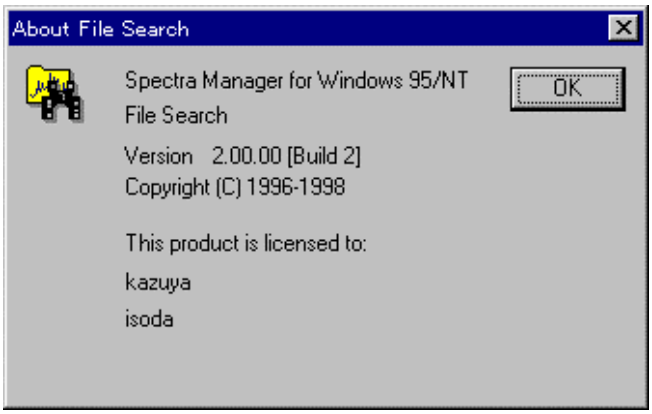


Fig. 3.8 [About File Find] dialog box

3.2.1 [Search Condition] dialog box

File searches are conducted using the [Search Condition] dialog box. Search parameters such as, the file type, directory and drive as well as the date and other information can be specified.

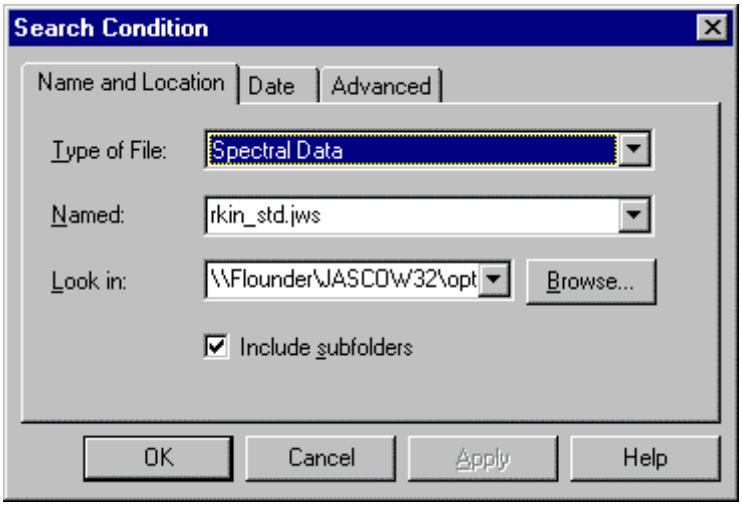


Fig. 3.9 [Search Conditions] dialog box showing the [Name and Location] tab

[Name and Location] tab

[Type of File] Select the type of file to be searched for. The following types are available:

JASCO Spectral Data Files
JASCO Mapping Data Files
JASCO Interval Scan Data Files

	JASCO DSC Data Files
[Named]	Specify the file name to be searched for. Wild card characters may be used (* means an unspecified string and ? means an unspecified character). For example, in the [Name] text box, type *.jws to search for all files with the jws extension.
[Look in]	Specify the drive and directory in which to search.
[Include subfolders]	Check to include all subdirectories beneath the currently selected directory in the search.
<OK>	Click to conduct the search according to the specified parameters(file type, directory, and drive). The results are displayed in the filename display area (see Fig. 3.3).

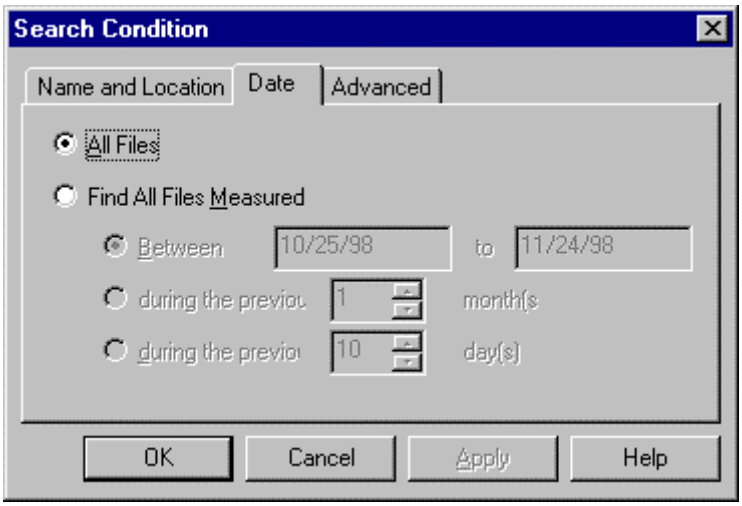


Fig. 3.10 [Search Conditions] dialog box showing the [Date] tab

[Date] tab

[All Files]	Select to search all files.
[Find All Files Measured]	Select to search files based on the option below.
[Between]	Searches for files measured within a set period of time.
[during the previous month(s)]	Searches for files measured within a specified number of months previously.
[during the previous day(s)]	Searches for files measured within a specified number of days previously.

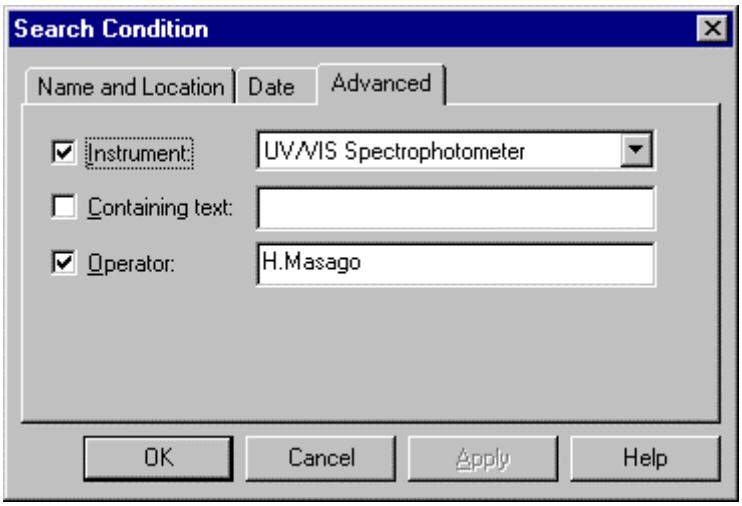


Fig. 3.11 [Search Conditions] dialog box showing the [Advanced] tab

[Advanced] tab

[Instrument]	Select to search for files measured using a specific instrument. Select the instrument from the drop-down list on the right. The instruments available are: Infrared Spectrometer Laser Raman Spectrometer UV/VIS Spectrometer Spectrofluorometer CD/ORD Ellipsometer
[Containing text]	Select to search for files that contain a particular portion of text in either the File name or Comments fields. Enter the text to search with in the text box on the right.
[Operator]	Select to search for files created by a specific operator.

4 Appendix

4.1 JCAMP-DX Format Files

The JCAMP-DX file format allows data conversion between various computers and media. The format was created by JCAMP (Joint Committee of Atomic and Molecular Physical Data). The program has the following characteristics:

- Format file data can be easily transferred between large computers, multi-purpose laboratory computers, common data processing systems, workstations, and personal computers.
- Because the format files are text files, the data can be viewed or edited using various commercially available editors.
- Peak tables and three-dimensional data can be handled in addition to spectra.

The V-500 can save measured and calculated data in JCAMP-DX format. Data saved in this format can be manipulated using the Grams data processing program or the Sadtler reference program. Although JCAMP-DX has several formats, only the V-500 format is explained here. Some knowledge of ASCII code is required in order to understand this explanation. A sample of JASCO's JCAMP-DX using Jasco FT as an example is given below.

```
##TITLE= Sample name    JCAMP-DX files always start with the ##TITLE= line.
##JCAMP-DX= 4.24        JCAMP-DX version
##DATA TYPE= INFRARED SPECTRUM        Designation for IR spectrum.
##ORIGIN= Jasco   Always Jasco.
##OWNER= Copyright(C)  Contents entered in [Copyright] in Jasco FT
##DATE= 96/08/17  Measurement date
##TIME= 13:33:46
##SPECTROMETER/DATA SYSTEM=Jasco Co. Ltd., Jasco FT for Windows, Ver. 1.00
##RESOLUTION= 4.000    Nominal resolution in units shown in ##XUNITS=.
##DELTAX= 1.92905045   Interval between data points (units in ##XUNITS=)
##XUNITS= 1/CM    Units of horizontal axis
##YUNITS= TRANSMITTANCE   Units of vertical axis (attribute)
##XFACTOR= 1.0000              Actual value is obtained by multiplying value in
                               ##XYDATA= by this factor.
##YFACTOR= 0.00001
##FIRSTX= 370.3777       First value for x-axis of ##XYDATA= (actual value)
##LASTX= 4627.7920       Last value for x-axis of ##XYDATA= (actual value)
##NPOINTS= 2208  Number of data points
##FIRSTY= 74.58664       Y-axis value corresponding to ##FIRSTX= (actual
        value)
##MAXY= 91.44050Maximum value of y-axis (actual value)
##MINY= 0.46792    Minimum value of y-axis (actual value)
##XYDATA= (X++(Y..Y))    Data are written from this point on
370.3777 7458664 7164965 6797073 6463581 6262086 6216446 6313309 6520278
385.8191 6759706 6993072 7203347 7370707 7518471 7794603 7953664
------(abbreviated)
4608.5015 8470810 8478381 8484588 8489256 8495972 8500248 8504088
4623.9341 8505672 85807172 8509182
##END=        JCAMP-DX files always end with the ##END= line.
```

4.1.1 JCAMP-DX file structure

4.1.1.1 LDR (Labeled-Data-Records)

LDRs consist of a data label (described later) and data. LDRs start with the ## data label flag and end with the next data label flag.

4.1.1.2 Lines

One line can contain up to 80 characters. The terminator for a line is CR-LF. LDRs can include several lines. Therefore, CR-LF does not necessarily designate the end of an LDR.

4.1.1.3 Data labels

A data label clarifies an LDR. Several labels are defined in the above example and further details are provided in Section 4.1.2. Data labels include the reserved labels defined by JCAMP as well as user defined labels that can record any information input by the user. The Jasco FT does not employ user-defined labels.

4.1.1.4 Blocks

A block is a set of LDRs starting with ##TITLE= and ending with ##END=. A single JCAMP-DX file can contain multiple blocks (the Jasco FT only responds to a one-block format).

4.1.2 Reserved labels

Only JCAMP-DX reserved labels that the Jasco FT can use are described here. Reserved labels that start with ##, and multiple labels cannot be placed on one line.

(1) ##TITLE=
All JCAMP-DX files start with ##TITLE= LDR. With the Jasco FT, the contents of [Sample Name] come after ##TITLE=.

(2) ##JCAMP-DX=
This LDR always comes after ##TITLE=. This shows the version of the file format.

(3) ##DATA TYPE=
Defines the data form of the block. This will always be an INFRARED SPECTRUM since only IR spectra can be saved using the Jasco FT.

Other ##DATA TYPES= include RAMAN SPECTRUM, INFRARED PEAK TABLE, INFRARED INTERFEROGRAM, and INFRARED TRANSFORMED SPECTRUM.

(4) ##ORIGIN=
Name and address of the file creator. Jasco is always entered here.

(5) ##OWNER=
Name of the owner of the spectrum. The contents of [Copyright] in the Jasco FT are entered here.

(6) ##DATA=, ##TIME=
Date (yy/mm/dd) and time (hh:mm:ss) of spectrum measurement.

(7) ##SPECTROMETER/DATA SYSTEM=
Records the measurement system and data processing system. This is always Jasco Corp., Jasco FT for Windows, Ver. 1.00.

(8) ##RESOLUTION=
Resolution in the units defined in ##XUNITS= (described later). This value differs from ##DELTAX= for data that have undergone zero filling.

(9) ##DELTAX=
Interval between data points expressed in the units defined in ##XUNITS=. As described above, this value differs from ##RESOLUTION= for data that have undergone zero filling.

(10) ##XUNITS=
Units of the horizontal axis. Since the Jasco FT cannot create JCAMP-DX files from interferograms, this value is always 1/cm (cm^{-1}). Other #XUNITS= include MICROMETERS, NANOMETERS, AND SECONDS.

(11) ##YUNITS=
Units of the vertical axis. The Jasco FT supports the following units (Abbreviations used in the Jasco FT are shown in parentheses):

TRANSMITTANCE (%T), REFLECTANCE (%R), ABSORBANCE (ABS), KUBELKA-MUNK (KM), ARBITRARY UNITS (other attributes).

(12) ##XFACTOR=, ##YFACTOR=
Data in ##XYDATA= become the actual values when multiplied by this factor.

(13) ##FIRSTX=, ##LASTX=
Value of the first and last data point on the ##XYDATA= horizontal axis (actual value).

(14) ##NPOINTS=
Number of ##XYDATA= data points.

(15) ##FIRSTY=
Value of the vertical axis at the ##FIRSTX= point (actual value).

(16) ##MAXY=, ##MINY=
Maximum and minimum values of the vertical axis (actual values).

(17) ##XYDATA=
Data are written from this point. The form of the data is (X++(Y..Y)). The first part of the line is the X-axis data and the following numbers to CR-LF are the Y-axis data.

In the previous example, 370.3777, 385.8101, etc. are wavenumbers. 7458664 is the datum at 370.3777 cm^{-1} and 7164965 is the datum at (370.3777 + ##DELTAX) cm^{-1} (for

the actual values, the various numbers must be multiplied by the factor in ##YFACTOR=). Although JCAMP-DX also has several other data formats, the Jasco FT handles only this format.

(18) ##END=
All JCAMP-DX blocks end with ##END=.

4.1.3 User-defined labels

In addition to the labels reserved by JCAMP-DX, users can create new labels. These labels are called user-defined labels. User-defined labels start with a $. The Jasco FT cannot output user-defined labels.

4.1.4 Adding comments

(1) ##=
Comments starting with this label can occupy any number of lines up to the next ## data label flag.

(2) $$
Comments starting with $$ can be placed anywhere on a line. This type of comment can only continue to the end of the line and does not designate the end of the LDR.

4.2 Smoothing Methods

Smoothing is intended to eliminate noise components from a spectrum to improve the signal-to-noise ratio. It is important that the optimum method is selected according to waveform because smoothing may distort signal components.
Four types of smoothing systems are available with the Spectrum Analysis program. The moving average method is an averaging method that assigns an appropriate weight to the measuring point of interest and the measuring points before and after that point.

1. Moving average
This method is used when the spectrum bandwidth is wide, that is, when the signal component is sufficiently smooth compared with noise.
The simple moving average method uses a rectangular coefficient as a weight function and the smoothing effect is high, but signal distortion is high.

2. Savitzky-Golay method
This method can be used to eliminate noise from most spectra.
It uses the weight coefficient[2)] given by Savitzky and Golay. The weight function changes based on the data width (convolution width) setting used in the smoothing.

3. Adaptive smoothing method
This method can be used conveniently to eliminate noise from a sharp spectrum such as a gas spectrum.
The spectrum is hardly distorted in the peak area and the smoothing effect can be enhanced in the baseline area by considering a coefficient based on noise dispersion and local signal dispersion.

4. Binomial method
In this smoothing method, the weight coefficient is given by a binomial coefficient. Compared with the Savitzky-Golay method, the binomial method has a number of

advantages such as the entire waveform is not distorted, phase (peak position) does not shift, and processing time is short.

Reference Literature

1) R.S.McDonald, P.A.Wilks Jr., Appl. Spectrosc. 47, 151(1988)
2) A. Savitzky, M.Golay, Anal. Chem. 36, 1627(1964)
3) P. Marchand, L. Marmet,Rev. Sci.Instrum. 54, 1034(1983)

4.2.1 Moving average method

The operating principle of the moving average method is based on a convolution calculation, similar to that of an analog filter.
The output *y(t)* of an analog filter is expressed by the following equation due to convolution of the input signal *x(t)* and filter impulse response *h(t)*.

$$y(t) = \int_{-\infty}^{\infty} x(\tau) \cdot h(t-\tau) d\tau = \int_{-\infty}^{\infty} h(\tau) \cdot x(t-\tau) d\tau$$

In the moving average method, the input signal is expressed by discrete values *x(i)* of *n* number (where *i*=1,2,....*n*) and so the smoothed value *y(i)* is determined as shown below by using a ″weight function″, *w(j)*, consisting of *N* (=2*m* +1) discrete points (where, *j* = -*m*, ... -1, 0, 1, ..., *m*).

$$y(i) = \frac{1}{W} \sum_{j=-m}^{m} w(j) \cdot x(i+j) \qquad : i = m+1, m+2, ..., n-m$$

$$W = \sum_{j=-m}^{m} w(j)$$

where *W* is a constant for normalization.

4.2.2 Simple moving average method

This is the simplest smoothing method and uses a rectangular function as a weight function. Given that the width of the rectangle is *N* = 2*m* + 1, the operating expression is given as follows.

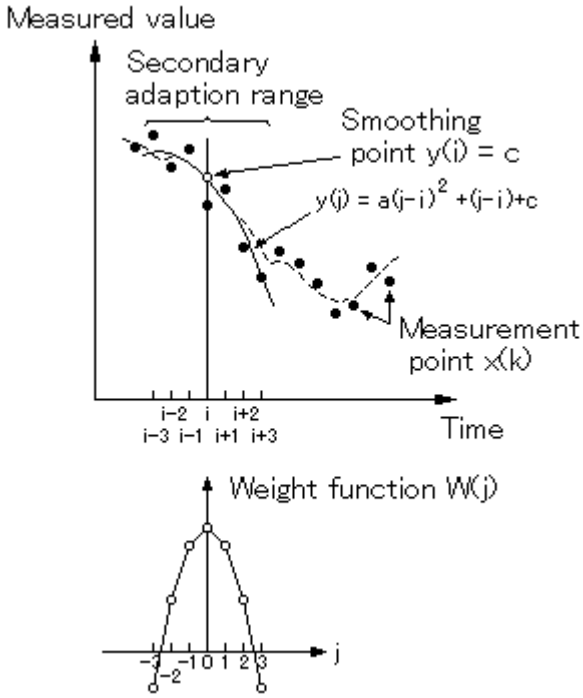
$$y(i) = \frac{1}{N} \sum_{j=-m}^{m} x(i+j) \qquad : i = m+1, m+2, ..., n-m$$

4.2.3 Savitzky-Golay method

This is a method of adapting the measurement waveform to a polynomial curve, based on the minimum square error norm in the neighborhood of each sample point. This method assumes that the measurement waveform can be expressed by a polynomial curve in its neighborhood. The type of weight function varies with the order of polynomial. A detailed table of values (weight coefficients) at each discrete point of this weight function was first reported by Savitzky and Golay. Therefore, the smoothing operation can be performed simply by performing convolution using this coefficient table.

Discrete point No.	25	23	21	19	17	15	13	11	9	7	5
-12	-253										
-11	-138	-42									
-10	-33	-21	-171								
-9	62	-2	-76	-136							
-8	147	15	9	-51	-21						
-7	222	30	84	24	-6	-78					
-6	287	43	149	89	7	-13	-11				
-5	342	54	204	144	18	42	0	-36			
-4	387	63	249	189	27	87	9	9	-21		
-3	422	70	284	224	34	122	16	44	14	-2	
-2	447	75	309	249	39	147	21	69	39	3	-3
-1	462	78	324	264	42	162	24	84	54	6	12
0	467	79	329	269	43	167	25	89	59	7	17
1	462	78	324	264	42	162	24	84	54	6	12
2	447	75	309	249	39	147	21	69	39	3	-3
3	422	70	284	224	34	122	16	44	14	-2	
4	387	63	249	189	27	87	9	9	-21		
5	342	54	204	144	18	42	0	-36			
6	287	43	149	89	7	-13	-11				
7	222	30	84	24	-6	-78					
8	147	15	9	-51	-21						
9	62	-2	-76	-136							
10	-33	-21	-171								
11	-138	-42									
12	-253										
Normalization coefficient	5175	805	3059	2261	323	1105	143	429	231	21	35

This is a coefficient table by adaptation of quadratic equation. The figure below shows the principle of smoothing using seven discrete points.



In this method, it is assumed that the signal waveform *y(j)* is expressed by the secondary equation below at each point *j* between 2*m*+1 points (the seven points in the above figure) around 1.

$$y(j) = a(j-i)^2 + b(j-i) + c \quad : j = -m+i,...,-1+i,i,1+i,...,m+i$$

Here, coefficients *a*, *b* and *c* are the square error in the secondary equation, where the square error from the actually measured value *x(j)*:

$$\sum_{j=-m+i}^{m+i} \{x(j) - y(j)\}^2$$

is minimum and can be calculated by the least squares method. At this time, the secondary equation adaptive value *y(i)* at the center point *i* is 0. The coefficient table contains weight coefficients used to determine coefficient *c*. Therefore, the smoothed value *y(i)* at point *i* is calculated as follows.

$$y(i) = \frac{1}{W} \sum_{j=-m}^{m} x(i+j) w(j)$$

$$W = \sum_{j=-m}^{m} w(j)$$

using the measurement value *x(j)* for 2*m*+1 points around this point and the value *w(j)* in the coefficient table (where, *j* = -*m*,...-1,0,-1...m)

4.2.4 Adaptation smoothing method

Let us assume that the measured waveform *x(i)* can be expressed by the sum of signal components *(i)* and the noise component *n(i)*:

$$x(i) = s(i) + n(i)$$

Let us also assume that noise *n(i)* is an irregular static noise (i.e. noise that does not change with time) having an average value 0 and dispersion σ_n^2, and that the signal is also static within a short time division. Here, the estimated value of the signal that

satisfies the minimum least square error norm is given as $\hat{s}(i)$. That is, $\hat{s}(i)$ is the value that minimizes $E\left\{\left(\hat{s}(i) - s(i)\right)^2\right\}$ and is given by the following.

$$\hat{s}(i) = \frac{\sigma_x^2(i) - \sigma_n^2}{\sigma_x^2(i)}\left\{x(i) - \bar{x}(i)\right\} + \bar{x}(i)$$

$$\bar{x}(i) = E\left\{x(i)\right\}$$

$$\sigma_x^2 = E\left\{\left(x(i) - \bar{x}(i)\right)^2\right\}$$

(Strictly speaking, E {} represents an aggregate average, but here it is given as a local average in the time base *i* direction.)

Noise dispersion σ_n^2 is determined by actual measurement. $\bar{x}(i)$ is determined by a simple moving average with constant width *N* and the estimated value of the true signal component can be obtained by calculating the dispersion $\sigma_x^2(i)$ of the measurement waveform in this width.

4.2.5 Binomial method

This is one of the moving average methods and is characteristic in that it can be realized by very simple operation and no hunting appears after smoothing. Smoothing is performed by repeat operation using the following equation a designated number of times.

$$y(i) = \frac{1}{4}(x(i-1) + 2 \times x(i) + x(i+1))$$

The table below gives the ″weight function″ *w(j)* with respect to the number of cycles and normalizing constant *W*. Compared with the Savizky-Golay method that performs polynomial approximation, this method is characteristic in that no negative values appears in the weight function. Thus, hunting does not occur in the neighborhood where input changes abruptly.

Discrete point No.	12	11	10	9	8	7	6	5	4	3	2	1
-12	1											
-11	24	1										
-10	276	22	1									
-9	2024	231	20	1								
-8	10626	1540	190	18	1							
-7	42504	7315	1140	153	16	1						
-6	134596	26334	4845	816	120	14	1					
-5	346104	74613	15504	3060	560	91	12	1				
-4	735471	170544	38760	8568	1820	364	66	10	1			
-3	1307504	319770	77520	18564	4368	1001	220	45	8	1		
-2	1961256	497420	125970	31824	8008	2002	495	120	28	6	1	
-1	2496144	646646	167960	43758	11440	3003	792	210	56	15	4	1
0	2704156	705432	184756	48620	12870	3432	924	252	70	20	6	2
1	2496144	646646	167960	43758	11440	3003	792	210	56	15	4	1
2	1961256	497420	125970	31824	8008	2002	495	120	28	6	1	
3	1307504	319770	77520	18564	4368	1001	220	45	8	1		
4	735471	170544	38760	8568	1820	364	66	10	1			
5	346104	74613	15504	3060	560	91	12	1				
6	134596	26334	4845	816	120	14	1					
7	42504	7315	1140	153	16	1						
8	10626	1540	190	18	1							
9	2024	231	20	1								
10	276	22	1									
11	24	1										
12	1											
Normalization constant	16777216	4194304	1048576	262144	65536	16384	4096	1024	256	64	16	4

4.3 Application of the self-deconvolution method

The Fourier self-deconvolution method is used to precisely distinguish the peak positions of each band in measurement spectra made up of multiple bands having the deconvolution method.

(1) The program requires that Lorentzian curves can be assumed for the spectral profile.

(2) The peak position of each band is the only representation of the shape after processing.
The reason for this is the vertical axis information of the spectrum is sacrificed in order to elucidate the horizontal axis information.

(3) The program cannot be applied to measurement spectra consisting of bands with differing widths, If the halfwidth of a band is taken as s' and the halfwidth of the deconvolution filter is taken as s, excessive deconvolution will occur when s>s' and insufficient deconvolution will occur when s<s'.

(4) When the signal-to-noise ratio of the measurement spectrum is poor, the signal-to-noise ratio after processing will deteriorate remarkably because, as with differential operations, the deconvolution filter emphasizes the high frequencies.

Principles

The program is an improved version of both the FSD (Fourier self-deconvolution) method proposed by Kauppinen et. al. and the FIRO (Finite Impulse Response Operator) method formulated by Jones and Shimokoshi. Both methods can be explained in principle by the FSD method, so the FSD method will be described here.

When the real spectrum is taken to be $E(\nu)$ the measured spectrum $M(\nu)$ is generally a shape "distorted" by instrumental function $G(\nu)$ of the measurement system. If the system is linear, the following equation can be expressed:

$$M(\nu) = G(\nu) * E(\nu) \tag{1}$$

Here the * symbol expresses the convolution integral. If $I_M(x)$ and $I_E(x)$ are taken to be the inverse Fourier transformation for $M(\nu)$ and $E(\nu)$, the equation becomes the following:

$$I_E(x) = \frac{1}{F^{-1}\{G(\nu)\}} I_M(x) \tag{2}$$

where $F^{-1}\{G(\nu)\}$ is the inverse Fourier transformation of $G(\nu)$. In other words, this shows the ideal inverse filter in the interferogram region. This filter is extremely sensitive to noise, so an apodization function $D(x, L)$ is introduced into equation (2) to cut or remove the high frequency noise with the FSD method.

$$I_E(x) = \frac{D(x, L)}{F^{-1}\{G(\nu)\}} I_M(x) \tag{3}$$

where *L* is the high frequency to be eliminated. The half width of $G(\nu)$ is assumed to have Lorentzian curve s. Therefore equation (3) becomes the following:

$$I_E(x) = \frac{D(x, L)}{\exp\{\pi\sigma|x|\}} I_M(x) \tag{4}$$

By performing a Fourier transformation on equation (4), the deconvoluted profile $E(\nu)$ can be obtained.

$$E(\nu) = F\left\{\frac{D(x, L)}{\exp\{\pi\sigma|x|\}} I_M(x)\right\} \tag{5}$$

These are the principles of the FSD method. Equation (5) can be converted into the following.

$$E(\nu) = F\left\{\frac{D(x, L)}{\exp\{\pi\sigma|x|\}}\right\} * M(\nu) \tag{6}$$

The FIRO method involves expanding the $\exp\{\pi\sigma|x|\}$ in equation (6) on the spectrum region for various types of apodization functions $D(x, L)$.

In this program, in order to reduce calculation time, an algorithm which mixes the FSD and FIRO methods is used. The deconvolution filter that is ultimately used on the spectrum has the following form:

$$F\left\{\frac{D(x, L)}{\exp\{\pi\sigma|x|\}}\right\} * D'(\nu, FL)$$

where $D(x, L)$ and $D'(\nu, FL)$ are both fixed to the Bessel function, and *L* and *FL* are handled with automatically determined values.

References

1) Appl. Spectrosc. 35, 271(1981).
2) Appl. Spectrosc. 37, 59(1983).

4.4 Phosphorescent lifetime

When the fluorescence intensity at time 0 is expressed as I_0, fluorescence intensity at time t is expressed as Equation (1).

$$I_t = I_0 e^{-t/\tau} \quad (1)$$

Converting this equation into logarithmic form yields Equation (2).

$$\log I_t = \log I_0 \quad (t/\tau) \quad (2)$$

In Equation (2), $\log I_0$ is the y-intercept and $-1/\tau$ is the slope.
τ is defined as phosphorescent lifetime.
Standard error (StdErr) is expressed in Equation (3):

$$\text{StdErr} \quad [\Sigma(\log I_t^e \quad \log I_t^m)^2]^{1/2}/N \quad (3)$$

N Number of Data
$\log I_t^e$ Calculated value
$\log I_t^m$ Measured value

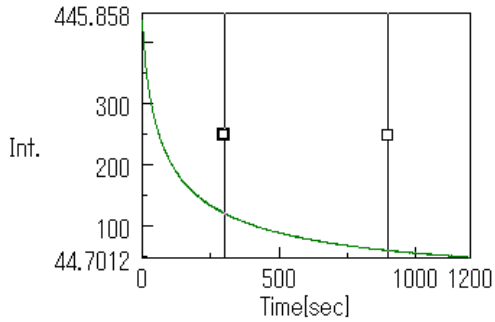


Fig. 4.1 Spectrum Data

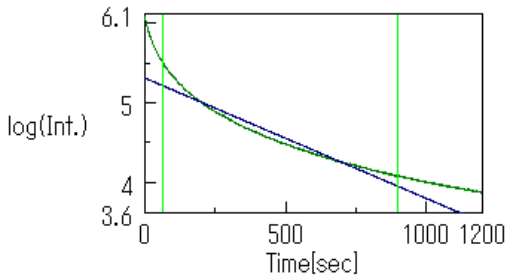


Fig. 4.2 Phosphorescent lifetime result