

**J-800 series**

# **CD Spectrometer**

**Software Operation Manual**

**Spectra Manager<sup>®</sup> Ver.2**



## Preface

This instruction manual serves as a guide for using this instrument. It is intended to instruct first-time users on how to properly use the instrument, and to serve as a reference for experienced users.

Before using the instrument, read this instruction manual carefully, and make sure you fully understand its contents. This manual should be easily accessible to the operator at all times during instrument operation. When not using the instrument, keep this manual stored in a safe place. Should this instruction manual be lost, order a replacement from your local JASCO distributor.

*Note: With this software you can use the same graphic user interface to analyze a wide variety of data from various spectroscopic instruments. This manual explains all the functions offered by this software using data from a JASCO spectrometer. We have tried to ensure that all functions are explained clearly for users of any JASCO instrument compatible with this software, but if you cannot find an explanation for a specific function please contact your local JASCO representative.*

## Servicing

Contact your local JASCO distributor for instrument servicing. In addition, contact your JASCO distributor before moving the instrument to another location. Consumable parts should be ordered according to part number from your local JASCO distributor. If a part number is unknown, give your JASCO distributor the model name and serial number of your instrument.

***Do not return contaminated products or parts that may constitute a health hazard to JASCO employees.***

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Modification of the software  
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- (3) The contents of this manual are subject to change without notice for product improvement.
- (4) This manual is considered complete and accurate at publication.
- (5) This manual does not guarantee the validity of any patent rights or other rights.
- (6) If a JASCO software program has failed causing an error or improper operation, this may be caused by a conflict from another program operating on the PC. In this case, take corrective action by uninstalling the conflicting product(s).

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# Contents

<i>Preface</i> .....	<i>i</i>
<i>Servicing</i> .....	<i>ii</i>
<i>Notices</i> .....	<i>ii</i>
<i>Limited Warranty</i> .....	<i>iii</i>
<i>Contents</i> .....	<i>v</i>
<b>1. General</b> .....	<b>1</b>
<b>1.1 About This Manual</b> .....	<b>1</b>
<b>1.2 Descriptions Covered by This Manual</b> .....	<b>2</b>
<b>1.3 Notations Used in this Manual</b> .....	<b>2</b>
<b>1.4 Program Window</b> .....	<b>3</b>
<b>2. Starting and Stopping Program and [Spectra Manager] Menu Reference</b> .....	<b>5</b>
<b>2.1 Starting the System</b> .....	<b>5</b>
2.1.1 Turn ON power to the J-800 CD Spectrometer .....	5
2.1.2 Starting Windows and the [Spectra Manager] Program .....	6
2.1.3 Starting a Measurement or Analysis Program .....	7
2.1.4 Cautions During Operation.....	8
<b>2.2 End</b> .....	<b>9</b>
2.2.1 Exit the Measurement and Analysis Program.....	9
2.2.2 Turning OFF Power to PC and Spectrometer .....	9
<b>2.3 [Spectra Manager] Menu Reference</b> .....	<b>10</b>
2.3.1 [Program] Menu .....	10
2.3.1.1 [Administrative Tools] .....	10
2.3.1.2 [Exit].....	10
2.3.2 [Application] Menu .....	11
2.3.2.1 [Start].....	11
2.3.2.2 [Open Parameter] .....	11
2.3.2.3 [Open Data] .....	12
2.3.2.4 [Information about Application] .....	12
2.3.3 [View] Menu.....	12
2.3.3.1 [Status bar] .....	12
2.3.3.2 [Folder].....	13
2.3.3.3 [Search] .....	13
2.3.4 [Help] Menu .....	13
2.3.4.1 [Contents].....	13
2.3.4.2 [Search Topic].....	13
2.3.4.3 [About...] .....	14
<b>2.4 [Administrative Tools] Menu Reference</b> .....	<b>15</b>
2.4.1 [Operation] Menu .....	15
2.4.1.1 [Install...] .....	15
2.4.1.2 [Register Instrument...].....	17
2.4.1.3 [Save List...] .....	18

2.4.1.4 [Exit...]	18
2.4.2 [View] Menu	19
2.4.2.1 [Status Bar...]	19
2.4.2.2 [Folder]	19
2.4.2.3 [Search]	19
2.4.3 [Help] Menu	19
2.4.3.1 [Contents]	19
2.4.3.2 [Search Topic]	19
2.4.3.3 [About...]	19
2.4.4 [Properties...] Menu	20
2.4.4.1 [Cell Unit]	21
2.4.4.2 [Composition]	23
2.4.4.3 [General]	24
2.4.4.4 [Adjustment]	25
2.4.4.5 [Photometry Mode]	26
<b>3. [Spectra Measurement] Menu Reference</b>	<b>27</b>
<b>3.1 [Measurement] Menu</b>	<b>28</b>
3.1.1 [Parameters...]	28
3.1.1.1 [General] Dialog Box	29
3.1.1.2 [Control] Dialog Box	32
3.1.1.3 [Information] Dialog Box	33
3.1.1.4 [Data] Dialog Box	34
<b>3.2 [Control] Menu</b>	<b>35</b>
3.2.1 [Select Accessory...]	35
3.2.2 [Move Wavelength...]	35
3.2.3 [CD Detector...]	36
3.2.4 [Light Source...]	36
3.2.5 [Shutter...]	37
3.2.6 [ORD-M Zero Clear]	37
<b>4. Practical Use of Spectra Measurement Program</b>	<b>38</b>
<b>4.1 Operation Overview of Spectra Measurement Program</b>	<b>38</b>
<b>4.2 Starting Spectrometer and Spectra Manager</b>	<b>38</b>
4.2.1 Starting Spectrometer	38
4.2.2 Checking the Registration of Accessories	38
<b>4.3 Measuring, Saving and Printing Spectra</b>	<b>39</b>
4.3.1 Sample Preparation	39
4.3.2 Starting the Spectra Measurement Program	39
4.3.3 Setting Parameters	40
4.3.4 Setting Sample and Measurement	42
4.3.5 Saving Spectra	44
4.3.5.1 Saving Parameters	44
4.3.5.2 Saving Baseline Data	45
4.3.5.3 Saving Sample Data	46
4.3.6 Transferring a Spectrum to [Spectra Analysis]	47
4.3.7 Printing Spectrum	47
<b>5. [Time Course Measurement] Menu Reference</b>	<b>48</b>

<b>5.1 [Measurement] Menu .....</b>	<b>50</b>
5.1.1 [Parameters...].....	50
5.1.1.1 [General] Dialog Box .....	50
5.1.1.2 [Control] Dialog Box.....	52
5.1.1.3 [Information] Dialog Box.....	54
5.1.1.4 [Data] Dialog Box .....	54
<b>5.2 [Control] Menu.....</b>	<b>56</b>
5.2.1 [Select Accessory...] .....	56
5.2.2 [Move Wavelength...].....	56
5.2.3 [CD Detector...] .....	57
5.2.4 [Light Source...].....	57
5.2.5 [Shutter...].....	58
5.2.6 [ORD-M Zero Clear].....	58
<b>6. Practical Use of Time Course Measurement Program.....</b>	<b>59</b>
<b>6.1 Operation Overview of Time Course Measurement Program.....</b>	<b>59</b>
<b>6.2 Starting instrument and Spectra Manager.....</b>	<b>59</b>
6.2.1 Starting Instrument .....	59
6.2.2 Checking the Registration of Accessories .....	59
<b>6.3 Measuring, Saving and Printing Data.....</b>	<b>60</b>
6.3.1 Sample Preparation.....	60
6.3.2 Starting the Time Course Measurement Program.....	60
6.3.3 Setting Parameters .....	61
6.3.4 Setting Sample and Measurement .....	63
6.3.5 Saving Data.....	65
6.3.5.1 Saving Parameters .....	65
6.3.5.2 Saving Sample Data .....	66
6.3.6 Sending Spectrum to [Spectra Analysis] .....	67
6.3.7 Printing Spectrum .....	67
<b>7 Operation of Spectra Analysis Program.....</b>	<b>68</b>
<b>7.1 Starting the spectra analysis program .....</b>	<b>68</b>
<b>7.2 Loading spectra.....</b>	<b>69</b>
7.2.1 Opening JASCO Standard file.....	69
7.2.2 Opening JASCO Old Std file.....	70
7.2.3 Saving as JASCO Standard file .....	70
7.2.4 Saving as JASCO Old Std file .....	71
<b>7.3 Calculation menus unique for the J-810/815 .....</b>	<b>71</b>
7.3.1 CD options .....	71
7.3.1.1 K-K conversion .....	71
7.3.1.2 HT -> OD .....	73
7.3.1.3 G-value .....	74
7.3.1.4 Optical Constant.....	75
7.3.2 Common Options.....	77
7.3.2.1 Channel Conversion .....	77
7.3.2.2 Data Dump .....	81
7.3.2.3 Data Accumulation.....	82
7.3.2.4 Arithmetic with Channel .....	82

7.3.2.5 Arithmetic with Data .....	85
<b>7.4 Closing Spectra Analysis Programs .....</b>	<b>87</b>
<b>8. Appendix .....</b>	<b>88</b>

# 1. General

## 1.1 About This Manual

This manual describes the configuration and operating procedure for the Model J-810/815 CD spectrometer which is operated using the Spectra Manager ver.2.0 program. It has eight sections, including this section (1. General). Each section contains the following information. Refer to “Spectra Analysis Program Instruction Manual” for the [Spectra Analysis] and [JASCO Canvas] programs. In this manual, Microsoft Windows 2000/XP Professional Edition is referred to as “Windows” and a personal computer as “PC”.

### 1. Introduction

Describes how to use this manual, notation used, and screen configuration. Read this section first.

### 2. Starting/stopping the program and [Spectra Manager] menu reference

Describes the procedures for turning ON the power to the J-800 and PC, starting Windows and the programs, exiting the programs and shutting down the PC and J-800. Using the information in this section become familiar with starting and shutting down the spectrometer. Refer to the following sections for information on program operation.

The menus in the [Spectra Manager] window that appear when the program is started are also described.

### 3. Introduction to the Spectra Measurement/Analysis program

#### 3 and 4. Spectra Measurement program reference

Section 3 describe the menus of the Spectra Measurement program. Read the relevant portions as required. Section 4 describes spectra measurement using the measurement program using simple examples. Those who are not familiar with Windows operation or who are not experienced in the operation of spectrometer should read this section and follow the instructions it gives. This section provides an overview of the J-800.

#### 3. [Spectra Measurement] menu reference

#### 4. Practical usage of [Spectra Measurement]

#### 5 and 6. Time Course Measurement program reference

This is for the Time Course measurement program.

#### 5. [Time Course Measurement] menu reference

#### 6. Practical usage of [Time Course Measurement]

### 7. The usage of special analysis functions for the J-810/815

### 8. Appendix

Contains suggestions on the setting of parameters and how to set up software and set the communication port. Refer to the relevant portions as required.

## 1.2 Descriptions Covered by This Manual

The J-800 program is an application program that runs under the Windows 2000/XP Professional Edition operating system. Therefore, a basic knowledge of Windows is required to use this program. This manual does not contain detailed information about the standard operation of Windows, such as using menus to run commands, copying of files, etc. First-time users of Windows should familiarize themselves with the standard operation of Windows by referring to the manual that comes with Windows.

## 1.3 Notations Used in this Manual

To aid comprehension, the following notations are used throughout this manual.

### General Notation

Notation	Meaning
[Measurement] menu [Parameters...] command	Names of menus, commands, and text boxes are enclosed in square brackets '[ ]', followed by a description indicating whether the function is a menu, command, text box, etc.
<OK>, <Cancel>	Names of buttons are enclosed in angular brackets '<>'.

### Keyboard Operations

Notation	Meaning
Shift CTRL	The key is enclosed in a square and shown in boldface.
Alt , F	Keys that are to be pressed in succession are separated by commas. In the example shown on the left, the "Alt" key is to be pressed and released, followed by the "F" key.
Shift + →	Keys that are pressed simultaneously are separated using the "plus" sign. In the example shown on the left, press the "→" key while holding down the "Shift" key.

### Mouse Operations

Notation	Meaning
Point	Move the mouse pointer to the specified item.
Click	Quickly press and release the mouse button.
Double-click	Click the mouse button twice in rapid succession.
Drag	Point to an item, click and hold down the mouse button. Move the mouse with the button held down, and release the button when the pointer is in the desired position.

## 1.4 Program Window

### (1) [Spectra Measurement] window

Names of the controls in the window are described below using the [Spectra Measurement] window as an example.

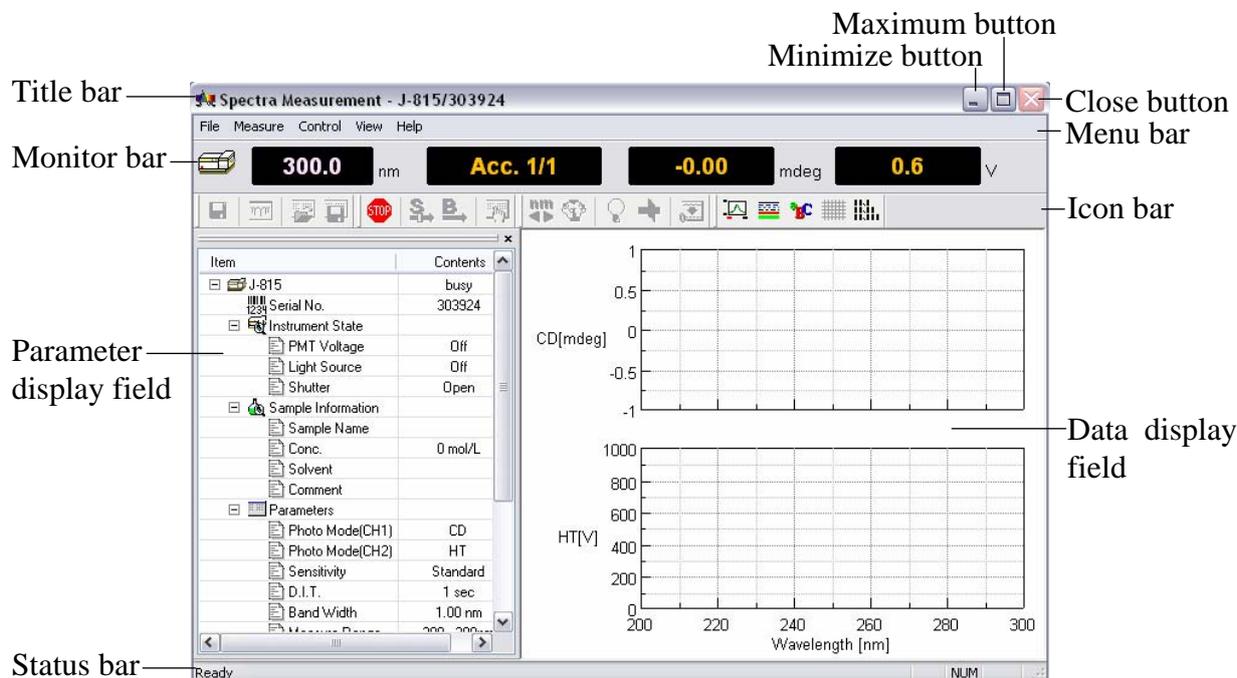


Figure. 1.1 [Spectra Measurement] window

Name	Function
Title bar	Displays the program name. The title bar in an active window (the window in which the operator is working) its appearance differs from other windows in color and brightness.
Menu bar	Displays the names of the menus that can be used. Each menu contains commands (operations) that can run.
Monitor bar	Displays the current wavelength, measured value and the operation button.
Status bar	Displays comments regarding the status of the spectrometer and the pull-down terms of the program window.
Data display field	Displays data, such as CD, HT, ORD, %T, Abs, etc.
Parameter display field	Displays the measurement parameters, sample information, spectrometer settings, etc.
Maximize button	Clicking on this button expands the active program window so that it fills the screen. In this state, the maximize button changes to a button that restores the window to its original size if clicked.
Minimize button	Clicking on this button minimizes the window.
Close button	Clicking on this button closes the window.

## (2) [Spectra Manager] window

This is the first window that appears when the [Spectra Manager] program in the [JASCO] menu is started (see Fig. 1.2). The menus of programs used by J-800 are displayed. From this window it is possible to control the operation of the spectrometer and program, transfer the data files into [Spectra Analysis], open graphs and information on the data file, display the directory of the data file, and open the [Administrative Tools], from which the communication port can be set up.

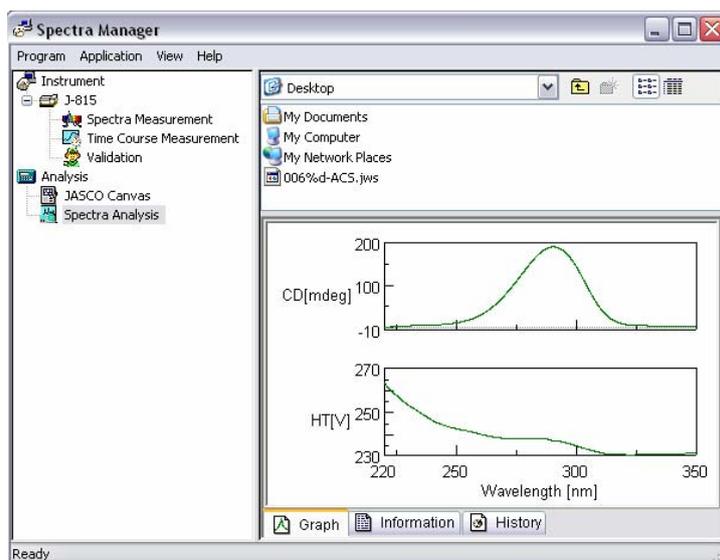


Figure. 1.2 [Spectra Manager] window

## (3) [Spectra Analysis] window

The [Spectra Analysis] program can open multiple windows to display data. This window is called a view (see Fig. 1.3). Multiple data can be incorporated in one view. Sending data from the measurement windows, [Spectra Measurement], [Time course measurement], or the [Spectra Manager] window, for example, starts the [Spectra Analysis] program and opens a view window and displays the measured data.

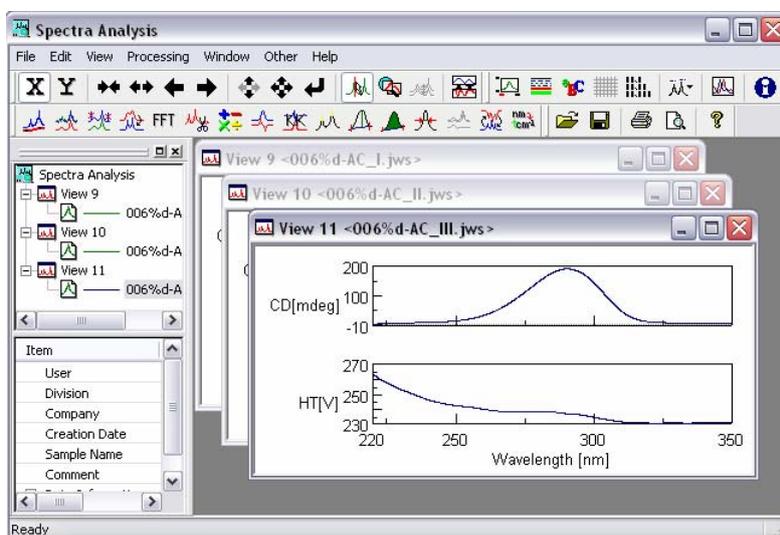


Figure. 1.3 [Spectra Analysis] window

**Note:** *In this manual, the analysis program is briefly summarized in Section 3. Refer to the operation manual for the spectrum analysis program for more information.*

## 2. Starting and Stopping Program and [Spectra Manager] Menu Reference

### 2.1 Starting the System

#### 2.1.1 Turn ON power to the J-800 CD Spectrometer

- (1) Make sure that the standard detector is installed on the J-800 CD spectrometer. If a long wavelength detector is installed, replace it with the standard detector. Refer to the hardware manual for how to remove and install the detector.
- (2) Feed nitrogen gas at a flow rate of 3 to 5  $\ell/\text{min}$ . It takes about five minutes to displace the interior of the optical system with nitrogen at this flow rate. If measurement is made at a wavelength shorter than 200 nm, the light will be absorbed by the small residual amount of oxygen present in air. In this case, increase the flow rate of the nitrogen so as to prevent the energy of the light incident on the sample from decreasing (See “CD ORD measurement manual” for details).

Measurement to 200 nm      3 to 5  $\ell/\text{min}$

Measurement to 185 nm      5 to 15  $\ell/\text{min}$

Measurement to 180 nm      15 to 20  $\ell/\text{min}$

Measurement to less than 180 nm      More than 20  $\ell/\text{min}$

**WARNING:** Running the xenon (Xe) lamp in air will generate ozone gas, which is harmful for humans. Turn on nitrogen gas flow at 3 to 5  $\ell/\text{min}$  a few minutes before turning on the light source.

**CAUTION:** Ozone gas absorbs light at wavelengths of 200 to 300 nm and 600 to 700 nm. This makes it difficult to take measurement in these wavelength regions and also will cause damage optical parts by corrosion. Always feed nitrogen gas before turning on the light source.

**CAUTION:** Never use helium gas. It will permeate into the photomultiplier tube, reducing the vacuum level and also its functionality of the photomultiplier tube.

**Note:** *If a PC-controlled nitrogen gas flowmeter (an optional accessory) is installed, all you need to do is simply open the main valve of the gas cylinder. Nitrogen will start flowing when the spectrometer is started. The flow rate can be controlled via the measurement program.*

- (3) With the 450 W Xe lamp, feed cooling water to the light source at a flow rate of about 2  $\ell$ /min.

**Note:** Step (3) above is not necessary for the 150 W Xe lamp, which is cooled with air.

- (4) Turn ON the "Power" switch at the front left bottom of the spectrometer.

**Note:** Just turning ON the "Power" switch does not result in the light source being turned on. The light source will be turned on automatically when the measurement program is started. (This function can be set in the [Administrative Tools] window (see Fig.2.23))

## 2.1.2 Starting Windows and the [Spectra Manager] Program

- (1) Starting PC and Windows 2000/XP Professional Edition.

Turn ON the power switches on PC and display, and start Windows. Refer to Windows 2000/XP Professional Edition manual for more information.

- (2) Starting Spectra Manager

Start [Spectra Manager] of [JASCO] according to the Windows starting procedure. The same operation can be performed by clicking the  button.

The Spectra Manager window appears (see Fig. 2.1).

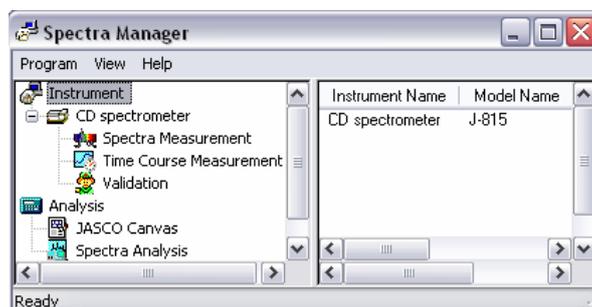


Figure. 2.1 [Spectra Manager] window

The [Spectra Manager] window displays the program menu used by the J-800 CD spectrometer. Fig. 2.2 shows the program menu for the standard spectrometer. Optional application programs, if any, can be added here. Refer to "2.3" [Spectra Manager] menu reference for more information about the [Spectra Manager] window.

**Note:** If multiple instruments are controlled by one PC, the J-800 icon may not be displayed in the [Spectra Manager] window. In this case, follow step (3) below.

- (3) Scroll down the [Instrument] window of Fig. 2.1 using the scroll bar.

### 2.1.3 Starting a Measurement or Analysis Program

- (1) Double-click the desired program from the displayed menu.

The program starts and the desired window appears after performing automatic procedures, *i.e.*, turning ON the light source (this depends on the properties set in [Administrative Tools]), initializing the spectrometer and program, transferring parameters, and moving the wavelength. It takes a while, which depending on the speed of the PC. When selecting the [Spectra Measurement] menu, for example, the following window appears (see Fig. 2.2)

**Note:** If a PC-controlled nitrogen gas flowmeter (an optional accessory) is installed, all you do is simply open the main valve of the gas cylinder. Nitrogen will start flowing when the spectrometer is started. The flow rate can be controlled at will on the measurement program.

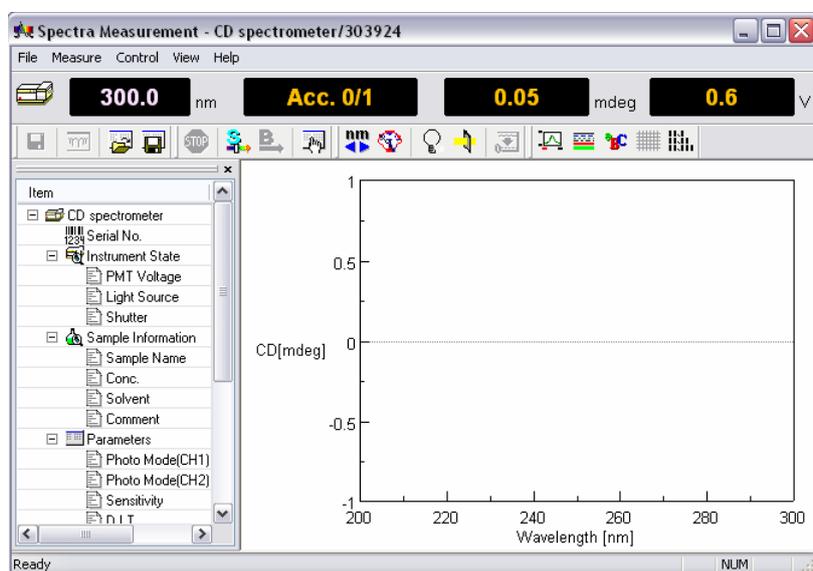


Figure. 2.2 [Spectra Measurement] window

**Note:** To verify whether the light source has been turned on or not check the "Lamp" LED on the amplifier panel on the front of the spectrometer.

If the light source does not light, the following warning message will appear (see Fig. 2.5). If this occurs, click on the <OK> button and turn ON the light by clicking the  icon which is located on the [Spectra Measurement] and the [Time Course Measurement] windows.



Figure. 2.3 Warning message for the light source

If the light source does not light or any error message is displayed, contact your local distributor along with [Error information of instrument].

**Note (1):** *If the light source temperature exceeds the normal level, a warning message will be displayed along with a buzzer alarm. In that event, take actions according to Table 2.1 "Corrective Actions against Errors".*

**Note (2):** *The alarm [Nitrogen flow rate low] <sup>\*)</sup> will appear if a PC-controlled nitrogen flowmeter or a nitrogen flowmeter with sensor is installed.*

**Note (3):** *If water leaks in the sample compartment, the user is alerted by an alarm and a buzzer <sup>\*)</sup>. Stop water supply, remove water, allow it dry up and eliminate the cause of water leakage.*

**Note (4):** *If the spectrometer is equipped with an optional water leak stop valve in the sample compartment, water will stop automatically when the water leak alarm goes off<sup>\*)</sup>.*

**Note (5):** *If the spectrometer will not be attended frequently during operation, it is recommended to provide a water leak stop valve in the sample compartment to minimize damage by water leakage.*

**Note (\*):** *This is available when appropriate settings are selected in the [condition] - [Properties...] - [Administrative Tools] - [Program] - [Spectra Manager] window. (Refer to "2.4").*

Table 2.1 Error Messages and Corrective Actions

<b>Error message</b>	<b>Corrective action</b>
Light source temperature high	Stop the spectrometer and restart operation. For the 450 W light source, increase the light source cooling water flow rate.
Light source cooling water flow rate low	Increase the light source cooling water flow rate.
Nitrogen flow rate low	Increase nitrogen gas flow rate. (Refer to "2.1.1")
Water leak in sample compartment	Refer to Notes (3) through (5) above.

### 2.1.4 Cautions During Operation

- (1) If the spectrometer is not attended for one hour or so, keep the light source lit. Turning ON/OFF the light source frequently will shorten its life.
- (2) If the slit width is set manually, do not widen the slit more than required. If it is widened excessively, the detector will be deteriorated sooner. Do not set the HT voltage (voltage applied to photomultiplier tube) below 170 volts.
- (3) If sample is spilt in the sample compartment, immediately wipe it off with gauze or the like.
- (4) If a sample or solvent that releases harmful gas is measured or if the humidity in the room is extremely high (more than 80%), install a sample compartment window to protect the monochromator. If measurement is made in a shorter wavelength region than 200 nm,

however, do not install the window.

- (5) Do not plug or remove the connector with the power turned ON. Failure can result.
- (6) The light source can be turned ON/OFF during operation. For the 450W light source, do not forget to stop light source cooling water when the light source is turned OFF. If cooling water is not stopped, dew will be condensed on the light source unit, causing deterioration of optical parts. Feed cooling water whenever the light source is lit.

## **2.2 End**

This section describes the procedure from existing the measurement and analysis program to turning OFF the power to the spectrometer and PC.

### **2.2.1 Exit the Measurement and Analysis Program**

- (1) To exit the spectrum analysis program, click on [File] - [Exit]. If data not yet saved exists or if the data on the disk is changed, it is reported a message to that effect. Take actions according to the message.
- (2) To exit the Spectra Measurement program, click on [Measure] - [Exit].
- (3) To exit the Spectra Manager, click on [Program] - [Exit]. [Spectra Manager] window closes, reverting to the Windows screen.
- (4) Exit Windows according to the manual for Windows 2000/XP Professional Edition.

### **2.2.2 Turning OFF Power to PC and Spectrometer**

- (1) Turn OFF the power to PC and display.
- (2) Turning off power to spectrometer
  - 1) Make sure that the sample compartment is empty of sample, turn OFF the "Power" switch on the spectrometer.
  - 2) If the 450W light source is used, stop its cooling water.
  - 3) Shut off nitrogen gas.

**CAUTION:** Stop cooling water whenever the light source is turned OFF. If cooling water is not stopped, dew will condense on the light source unit, deteriorating the optical parts.

## 2.3 [Spectra Manager] Menu Reference

The [Spectra Manager] window starts the program for making measurements and data analysis, selects, starts/stops and sets the communication port of the spectrometer and registers optional accessories.

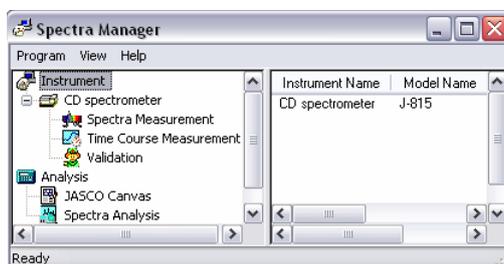


Figure. 2.4 [Spectra Manager] window

Fig. 2.4 shows the standard measurement/analysis program menu. It is added to this menu when an application program is installed. The left side shows the analysis menu and the right side shows information about the spectrometer including its name, model number, serial number, username, and its status. Double-clicking the menu starts the program. If the spectrometer program has not been started, they will start simultaneously.

### 2.3.1 [Program] Menu

#### 2.3.1.1 [Administrative Tools]

In this window, the communication port of the spectrometer can be set, and optional accessories can be registered, etc. Selecting the [Administrative Tools] menu displays the following window.

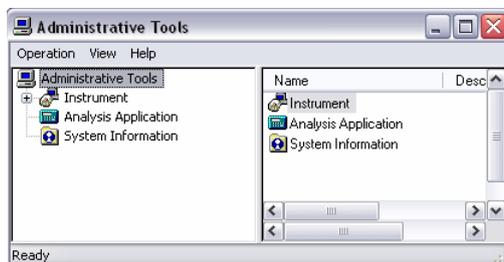


Figure. 2.5 An example for use of [Information about Application] box

Refer to “2.4” for details.

#### 2.3.1.2 [Exit]

This stops the [Spectra Manager] program and/or communication with the spectrometer.

**Note:** When the [Spectra Manager] program is exited, communication with the spectrometer is terminated automatically.

## 2.3.2 [Application] Menu

### 2.3.2.1 [Start]

This menu starts a measurement or analysis program.

- (1) Click the desired measurement or analysis program in the [Spectra Manager] window. (See Fig. 2.6)

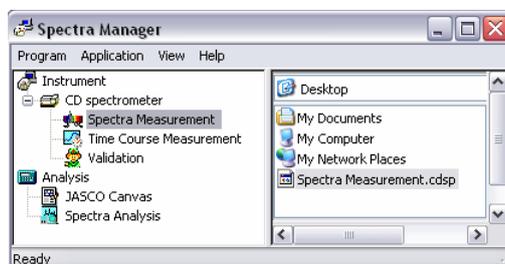


Figure. 2.6 Starting [Spectra Measurement] program

- (2) Select the [Start] - [Application] menu.

The program can also be started by double-clicking the measurement or analysis program name. Refer to the relevant manual for more information.

### 2.3.2.2 [Open Parameter]

This menu imports the measurement parameters to the spectrometer and starts the selected measurement program. Execute in the following manner.

- (1) Click the desired measurement program in the [Spectra Manager] window (see Fig. 2.6)
- (2) Search the directory and select the measurement parameter file (i.e. .cdsp format file) in the right side of the window. (See the right side of Fig. 2.7)

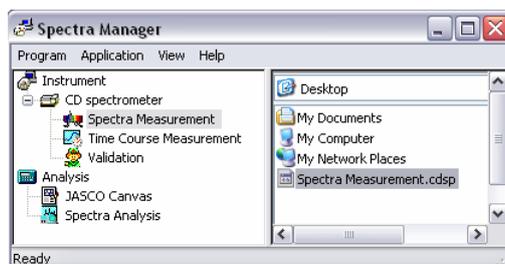


Figure. 2.7 Starting [Spectra measurement] program and reading parameters simultaneously

- (3) Select the [Open Parameters] - [Application] menu.

Procedure (3) is an alternative to double-clicking the .cdsp format file. The conditions and date of measurement are displayed in the lower right-hand section of the [Spectra Manager] window.

**Note:** The [Open Parameters] menu only opens measurement parameters, it can not be used for opening measurement results.

### 2.3.2.3 [Open Data]

This menu reads the measurement result and starts the [Spectra Analysis] programs. Execute in the following manner.

- (1) Click [Spectra Analysis] in the [Spectra Manager] window.
- (2) Search the directory and select a measurement result file (a .jws format file)

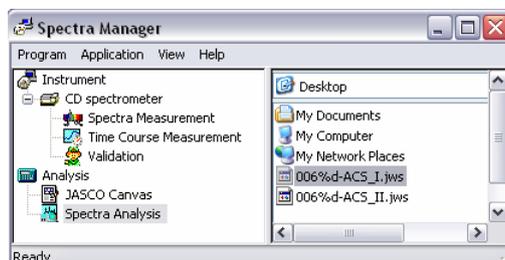


Figure. 2.8 Starting [Spectra Analysis] program and reading data simultaneously

- (3) Select the [Open Data] - [Application] menu.

Procedure (3) is an alternative to double-clicking the .jws format file. Spectra and information about the measurement including the date that the measurement was performed are displayed in the lower right-hand of the [Spectra Manager] window.

### 2.3.2.4 [Information about Application]

This menu displays information about the program. In the case of the [Spectra Measurement] program (see Fig. 2.6) the following dialog box is displayed.



Figure. 2.9 [Information about Application] dialog box

## 2.3.3 [View] Menu

### 2.3.3.1 [Status bar]

This displays or hides information concerning the pull-down menu.

- (1) Make the [Status Bar] - [View] menu active.
- (2) Use the cursor to point to the desired menu.

The following information is displayed when the [Start] - [Application] menu is selected.

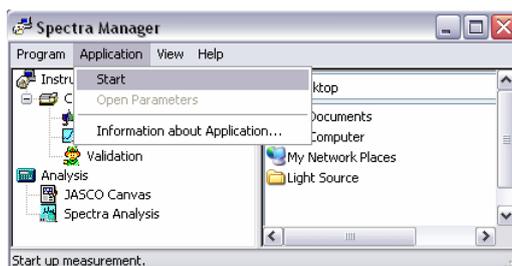


Figure. 2.10 The [Status Bar] description

### 2.3.3.2 [Folder]

Displays files on the right side of the [Spectra Manager] window.

### 2.3.3.3 [Search]

Locates data files and displays them on the right side of the [Spectra Manager] window.

## 2.3.4 [Help] Menu

### 2.3.4.1 [Contents]

Displays the operating procedure for Spectra Manager ver.2.

- (1) Selecting the [Contents] - [Help] menu will result in the following window being displayed.



Figure. 2.11 The [Contents] window

- (2) Click the [Forward] icon to go forward.
- (3) Click the [Back] icon, to go backward.

### 2.3.4.2 [Search Topic]

Search for help topics on the operation of Spectra Manager ver.2.

- (1) Select the [Search Topics] - [Help] menu and the following window is displayed.

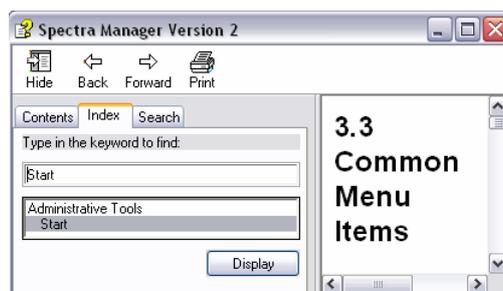


Figure. 2.12 The [Index] window

- (2) Select the [Start] menu, and click the <Display> button in Fig. 2.12.  
The window shown in Fig. 2.13 appears.

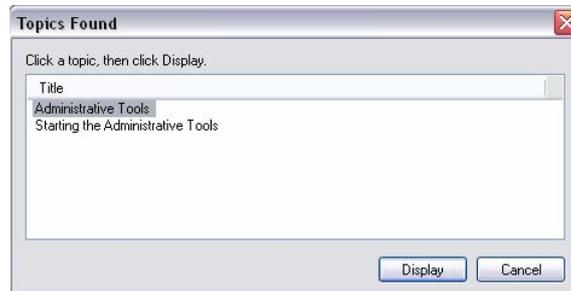


Figure. 2.13 [Help] dialog box

- (3) Selecting the [Administrative Tools] menu, for example, results in comments about it being displayed on the right side of the [Index] window (see Fig. 2.12).
- (4) Click the [Search] tab and enter a word into the column, to find the help topics concerning the word.

If you want to display a list of all of the topics:

- (5) Right-click the icon, [Hide], [Back], [Forward], or [Print] of Fig. 2.11 or Fig. 2.12 and select the [Open all] menu.

This will display all of the topics. Alternatively, all of the topics can be displayed by:

- (6) Right-clicking the icon, [Hide], [Back], [Forward], or [Print] of Fig. 2.11 or Fig. 2.12 and select the [Close all] menu and all of the topics will be displayed.

### Others

- (7) Click the [Hide] icon of Fig. 2.11 (or Fig. 2.12).

The left side of Fig. 2.11 (or Fig.2.12) is hidden.

- (8) Click the [Print] icon of Fig. 2.11 (or Fig. 2.12).

The comments displayed on the right side of Fig. 2.11 (or Fig. 2.12) will be printed out. The [Print] function can also be performed by right-clicking the icon, [Hide], [Back], [Forward], or [Print] of Fig. 2.11 (or Fig. 2.12) and then selecting the [Print...] menu.

### 2.3.4.3 [About...]

Displays information about Spectra Manager ver.2. (See Fig. 2.14)



Figure. 2.14 The dialog box that displays information about [Spectra Manager]

Click the <OK> button to return to the [Spectra Manager] window (see Fig. 2.4)

## 2.4 [Administrative Tools] Menu Reference

The [Administrative Tools] window's main function is installing programs, setting the environment of the spectrometer and registering spectrometers and optional accessories. When nothing has been installed, the [Administrative Tools] window appears as shown below.

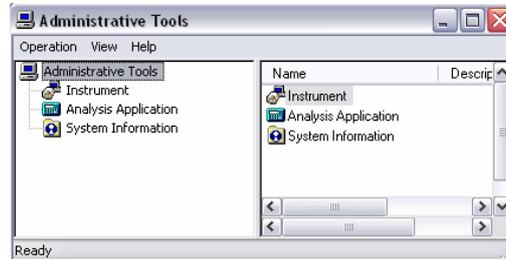


Figure. 2.15 [Administrative Tools] window

The details concerning the menus displayed on the left side of the window are displayed on the right side of the window.

### 2.4.1 [Operation] Menu

#### 2.4.1.1 [Install...]

This is for installing measurement and data analysis programs. The installation method using the [Spectra Analysis] program is described below.

- (1) Select the [Operation] - [Install...] menu.
- (2) Input the drive and name of the target [Spectra Analysis] program directory.



Figure. 2.16 Data directory input screen

The <Browse...> button is a convenient method for selecting the target program. In the case of Fig. 2.16, the following directory name was selected: E:\SpectraAnalysis\_201K.

**Note:** The target program should not be located on the desktop. A floppy disk, removable disk, or local disk drive C: are the most suitable.

- (3) Click the <Next> button.

The screen shown in Fig. 2.17 appears.

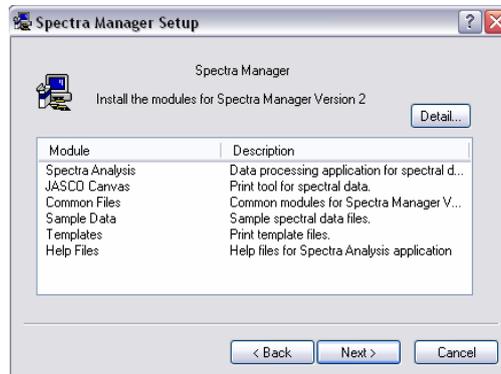


Figure. 2.17 The contents of [Spectra Analysis] program

Fig. 2.17 shows the contents of the program and their details.

- (4) Click the <Next> button.

This results in the installation being carried out and when installation has been completed Fig. 2.18 is displayed.

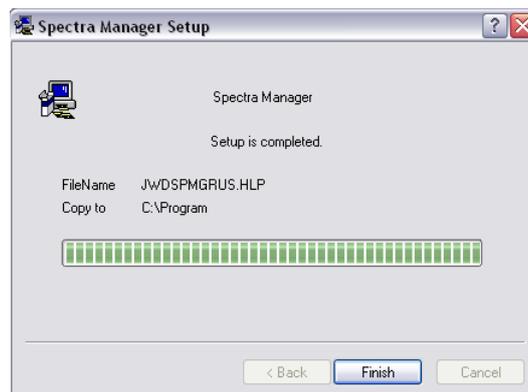


Figure. 2.18 The dialog box which showing that installation has been completed

- (5) Click the <Finish> button.

Doing this returns to the [Administrative Tools] window. Click the [Analysis Application] menu of the [Administrative Tools] window, and the contents of the [Analysis Application] program are displayed on the right side of the window (see Fig. 2.19).

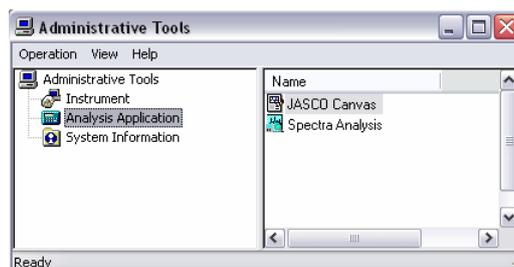


Figure. 2.19 [Administrative Tools] window after installation

**CAUTION:** *The [Spectra Analysis] program must be installed first. Once it has been installed other programs for the instruments and their accessories can be installed.*

**Note:** *If the programs are installed in a different order program they may not function correctly.*

#### 2.4.1.2 [Register Instrument...]

Registers the status when first using the spectrometer or an accessory.

**Note:** *Whenever an optional accessory is used, open this dialog box to register it. Accessories cannot be controlled using driver programs unless they are registered in this manner.*

- (1) Open the [Administrative Tools] window by selecting [Register Instrument...] - [Operation] after installing the standard J-800 driver (Refer to “2.4.1.1” concerning installation of programs).

The following screen appears.

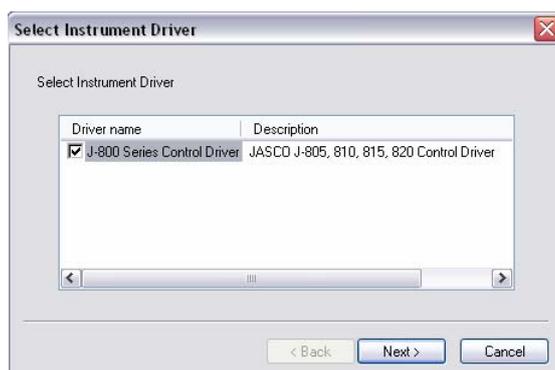


Figure. 2.20 The instrument registration screen

Clicking the <Cancel> button, returns to the previous [Administrative Tools] window.

- (2) Check the box as shown in Fig. 2.21 and click the <Next> button.

The following screen will appear.

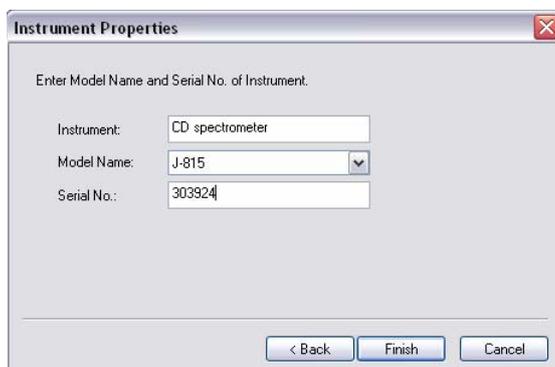


Figure. 2.21 Registration of serial No., model name and instrument name

Clicking the <Back> button and the <Cancel> button, reverts to the previous screen (see Fig. 2.20) and the [Administrative Tools] window, respectively.

(3) Enter the serial No., model name and instrument name in the given boxes.

**Note:** *The Serial No. is unique for each instrument. So the No. and the model name should be entered correctly. If they are entered incorrectly, access to the instrument will be denied.*

(4) Click the <Finish> button.

Doing this reverts to the [Administrative Tools] window. Click the [Instrument] menu of the [Administrative Tools] window and the contents of the program are displayed on the right side of the window (see Fig. 2.22).

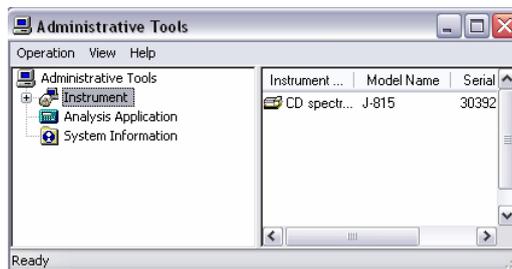


Figure. 2.22 [Administrative Tools] window after installation

#### 2.4.1.3 [Save List...]

Saves the contents that appear on the right side of the [Administrative Tools] window as a .txt format file. When clicking the [Instrument] menu (see Fig. 2.22) the following information is saved.

Instrument name	CD spectrometer
Model name	J-815
Serial No.	303924
Conditions	Waiting

These the above information is registered for the example depicted in Fig. 2.21.

#### 2.4.1.4 [Exit...]

Closes the [Administrative Tools] window.

## 2.4.2 [View] Menu

### 2.4.2.1 [Status Bar...]

Displays or hides the comments concerning the pull-down menus.

- (1) Make the [Status Bar] - [View] menu active.
- (2) Hover the cursor over the menu of interest.

The following information is displayed when the [Operation] - [Install] is selected.

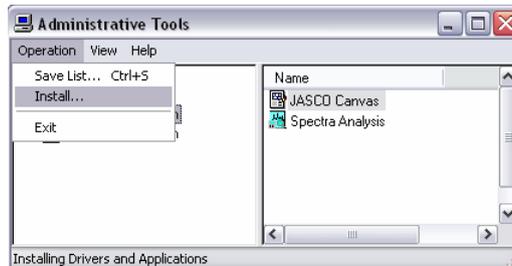


Figure. 2.23 [Status Bar] description

### 2.4.2.2 [Folder]

Displays files on the right side of the [Administrator Tools] window.

### 2.4.2.3 [Search]

Locates a data file and displays it on the right side of the [Administrator Tools] window.

## 2.4.3 [Help] Menu

### 2.4.3.1 [Contents]

Displays information about using [Administrative Tools], which is on-line help. Its usage is the same as for the [Contents] - [Help] menu (Refer to “2.3.4.1”).

### 2.4.3.2 [Search Topic]

Searches the topic list for the operations of the [Administrative Tools]. Its usage is the same as for the [Contents] - [Help] menu (Refer to “2.3.4.2”).

### 2.4.3.3 [About...]

Displays information about the [Administrative Tools] as shown below.



Figure. 2.24 The dialog box that displays information about Administrative Tools

Click the <OK> button, to return to the [Administrative Tools] window.

## 2.4.4 [Properties...] Menu

This is for registering optional accessories, setting, diagnosing, and initializing the spectrometer.

- (1) Select [Operation]-[Properties...] after confirming the name of the spectrometer (see Fig. 2.25).

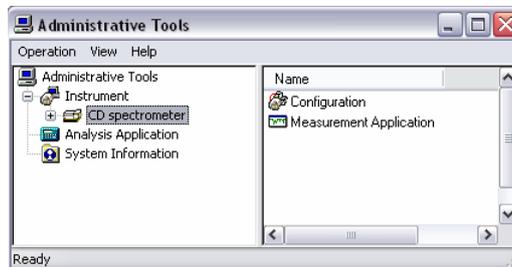


Figure. 2.25 Opening [Properties...]

The following dialog box is displayed.

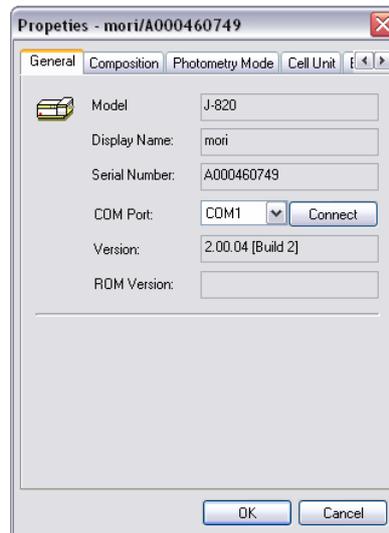


Figure. 2.26 [Properties...] dialog box

### 2.4.4.1 [Cell Unit]

This is for registering optional accessories.

- (1) Click the [Cell Unit] tab.

The following screen is displayed.

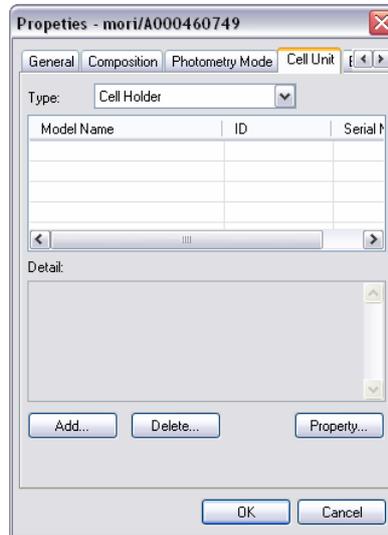


Figure. 2.27 [Cell Unit] dialog box

- (2) Select the optional accessory in the <Type> box.

Click the <Add...> button and the following dialog appears.



Figure. 2.28 Input screen

Clicking the <Cancel> button reverts to the dialog box shown in Fig. 2.27.

- (3) Select the Accessory ID and enter the serial No. and comment in the relevant boxes (see Fig. 2.28).

- (4) Click the <OK> button.

The contents are displayed as shown in Fig. 2.29.

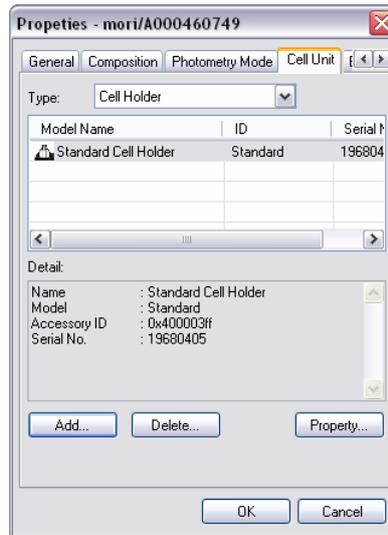


Figure. 2.29 Updated [Cell Unit] dialog box

Additional optional accessories can be registered by clicking the <Add...> button and following the steps (1) to (5). On the other hand, the accessories can be removed by selecting the name of the model to be deleted name as shown in Fig. 2.29 and then clicking the <Delete...> button.

- (5) Click the <OK> button.

The accessory is registered and it returns to the [Administrative Tools] window (see Fig. 2.25). If the <Cancel> button is clicked, no changes are effected.

**Note (1):** The optional accessories must be registered before using them to take measurements.

**Note (2):** Standard Cell Unit is an standard accessory.

### 2.4.4.2 [Composition]

Sets the status of the spectrometer when it is first used. Turn it on by inserting a check mark, if or when required.

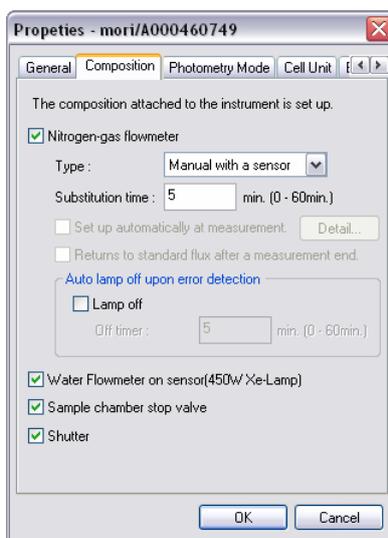


Figure. 2.30 [Composition] dialog box

**Note:** *Inserting a check mark in this dialogue box allows control of the shutter and varies the nitrogen flow rate in the measurement program.*

[Turn on light source at start] Turns the light source ON/OFF initially.

[Nitrogen flowmeter] Sets the parameters of the nitrogen flowmeter. If the spectrometer has a flowmeter, insert a check mark.

[With sensor] Select this option if using a nitrogen flowmeter with a sensor.

[PC control] Select this option when the nitrogen flowmeter is controlled by a PC.

[Idling time] Enter the time required between the commencement of nitrogen flow to turning on the light source.

[Light source cooling water flowmeter with sensor] Insert a check mark for the J-800 (450 W xenon lamp).

[Sample compartment leak water stop valve] Insert a check mark when the spectrometer has a sample compartment leak water stop valve (optional accessory).

[Shutter] Insert a check mark for J-800.

### 2.4.4.3 [General]

Displays information about the spectrometer and changes the communication port. The serial port COM1 is set as default (see Fig. 2.31).

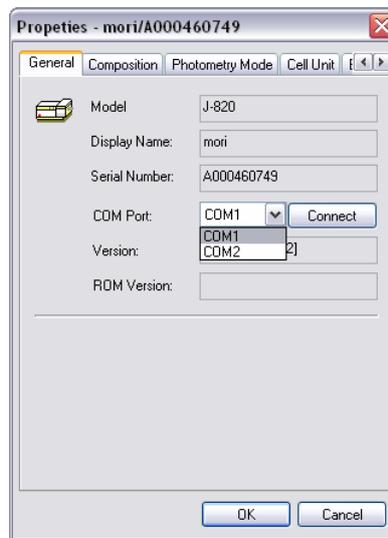


Figure. 2.31 [General] dialog box

The communication port can be changed by clicking the <Connect> and <OK> buttons after clicking on the desired port in the [COM Port] list.

**Note:** *The connection must be performed before diagnosing and/or initializing the spectrometer.*

#### 2.4.4.4 [Adjustment]

Diagnoses and initializes the spectrometer, and sets the Xe lamp to turn on automatically when a measurement is performed. The [Adjustment] tab screen shown below appears by connecting the port as shown in Fig.2.31.

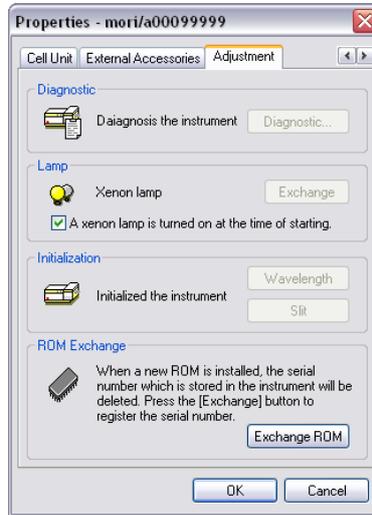


Figure. 2.32 [Adjustment] dialog box

CASE I: Diagnostic of the spectrometer

Click the < Diagnostic > button and the following dialog appears.

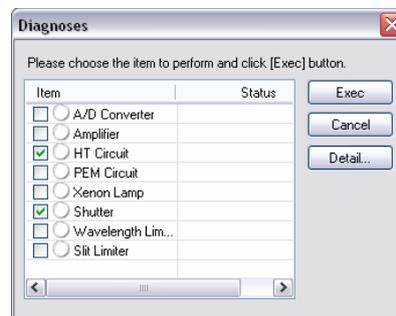


Figure. 2.33 [Diagnosis] dialog box

- (1) Put checkmarks next to the items to be diagnosed and click the <Exec> button (see Fig. 2.33)

Diagnosis is performed and the results appear as shown below.

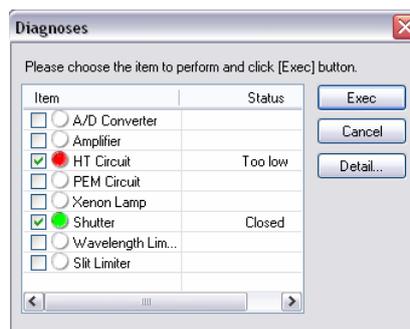


Figure. 2.34 [Diagnosis] dialog box after checking instrument

Clicking on the <Detail> button displays spectrometer error information.

**Note:** During diagnosis, the dialog box for each diagnosis appears. Wait for a while until the diagnoses are completed.

CASE II: Initialization of the spectrometer

Initializes the wavelength and slit drives.

**Note:** During initialization, the dialog boxes for the wavelength and slit drives appear. Wait for a while until the initializations are completed.

CASE III: Several settings of Xe lamp

Sets the Xe lamp to turn on automatically and initializes the number of hours that the Xe lamp has been used. The former is set by checking the appropriate check boxes while the latter is performed by clicking the <Exchange> button.

**Note:** A password is necessary for initializing the number of hours that the Xe lamp has been used. The password is 0426464111.

CASE III: ROM Exchange

Over write the old serial number with registered one (depicted in Fig.2.21, for example).

**CAUTION:** [ROM Exchange] is set for service engineer of JASCO and its groups. This function must not be used since the ROM may be destroyed.

#### 2.4.4.5 [Photometry Mode]

Select the following menu when using corresponding accessories. Selected items are added into [Photometry Mode] of the measurement programs.

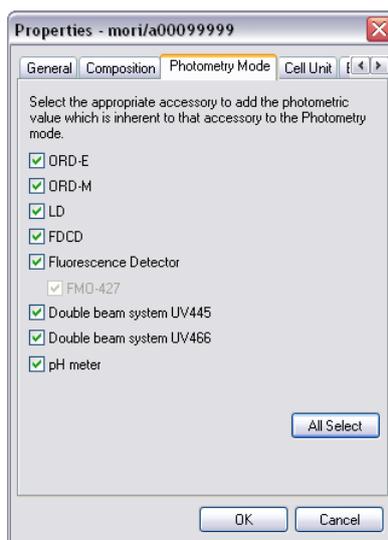


Figure. 2.35 [Photometry Mode] dialog box

### 3. [Spectra Measurement] Menu Reference

Starting the Spectra Measurement program displays the following window.

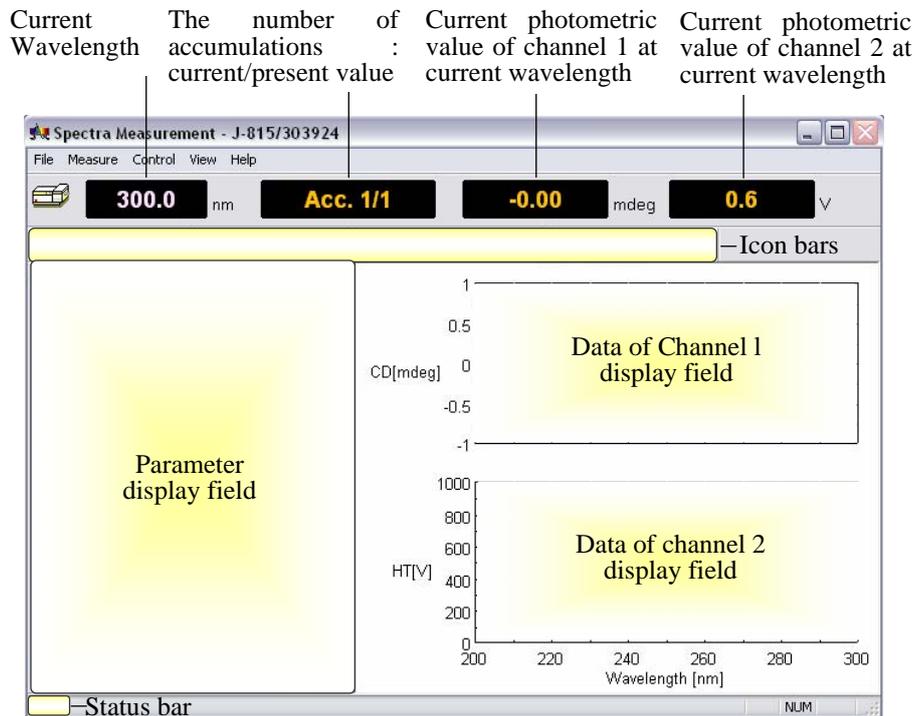


Figure. 3.1 [Spectra Measurement] window

**Note:** The program can display up to four types of data simultaneously by changing the number of measuring channels.

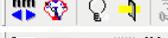
#### [File] menu

- |                      |   |
|----------------------|---|
| [Save Data...]       | Saves experimental setup data, measurement parameters, and set terms as a .jws format file.                               |
| [Analysis Send]      | Transfers experimental data to the [Spectra Analysis] window, which starts up automatically when [Analysis Send] is used. |
| [Open Baseline...]   | Opens baseline data file, which are .cdsl format files.   |
| [Save Baseline...]   | Saves baseline data to disk as .cdsl format files.  |
| [Open Parameters...] | Opens parameters which are set in the [Parameter Settings] dialog box. The file format is .cdsp.                          |
| [Save Parameters...] | Save parameters as a .cdsp format file.   |
| [Exit]               | Exits the [Spectra Measurement] window.   |

#### [Measure] menu

- |                 |   |
|-----------------|---|
| [Parameters...] | Sets parameters, turns [Baseline] measurements and auto-shutter control ON/OFF, edits comments and saves and loads measurement parameters and data. |
| [Sample]        | Starts measurement of sample.   |
| [Baseline]      | Starts [Baseline] measurement.  |
| [Cancel]        | Stops blank and sample measurement.   |

#### [Control] menu

[Move Wavelength...]	Moves the current wavelength to desired value.
[CD Detector...]	Sets detector (CD/ORD/LD/UV) sensitivity.
[Light Source...]	Turns the light source ON/OFF. Displays/clears the light source operating time.
[Shutter...]	Opens or closes the shutter (when installed).
[Auto Zero]	Zeroes the photometric value of ORD-M (when installed).
[Accessory...]	Registers compatible accessories.
<b>[View] menu</b>	
[Select Graph...]	Selects the desired channel No. (default is channel 1).
[Overlay]	Overlay the graphs.
[Scale...]	Sets the minimum and maximum values for the vertical and/or horizontal axes/axis.
[Pattern...]	
[Font...]	Sets the font type for the axes values and/or unit(s).
[Grid...]	Displays or hides grid.
[Style...]	Sets the scale interval.
[Select Graph...]	Selects which graphs are displayed or hidden.
[Information Bar]	Displays or hides parameters such as those shown in Fig. 4.1.
[Toolbar...]	Displays or hides the toolbars shown in Fig. 4.1.
[File]	Displays or hides the toolbar:  .
[Measure]	Displays or hides the toolbar:  .
[Control]	Displays or hides the toolbar:  .
[View]	Displays or hides the toolbar:  .
[Status Bar...]	Displays or hides the status bar of Fig. 4.1.
[Customize Toolbar...]	Selects the icons to be displayed and defines the appearance of the toolbar.
<b>[Help] menu</b>	
[Contents]	Displays the contents of the instrument.
[About...]	Displays the version and copyright.

## 3.1 [Measurement] Menu

### 3.1.1 [Parameters...]

Sets parameters, turns shutter ON/OFF for blank measurements and auto-shutter drive, edits comments and saves and loads measurement parameters and data onto or from disk. The parameters dialog box is made up of four dialog boxes: [General], [Control], [Information] and [Data]. They can be changed by clicking the appropriate tab at the top of the box. Clicking the tab [Data], for example, when the [Parameters Settings] dialog box is active displays the [Data] dialog box. The dialog boxes are described below.

### 3.1.1.1 [General] Dialog Box

Sets the parameters of the spectrometer.

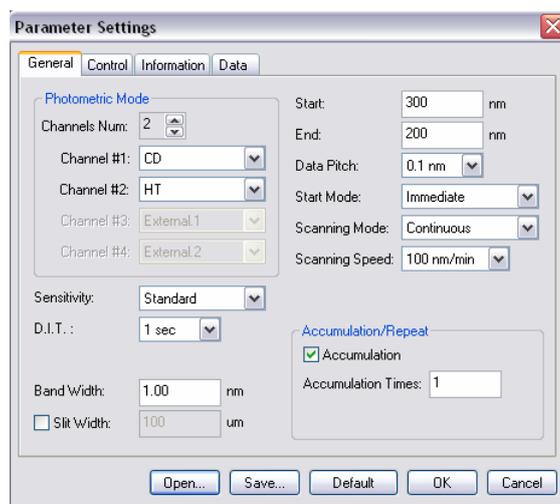


Figure. 3.2 [General] dialog box

#### Photometric mode

[Channel Num] Maximum of four channels. Four types of data can be acquired simultaneously.

[Channel #1] The selectable range varies with an optional accessory.

CD: Circular dichroism signal, which is given by  $\sim AC/DC$  with 50 kHz.

CD/DC: This is the same with CD mode when DC is set to 1 V. This mode is useful when the DC varies (i.e., HT is fixed at an arbitrary value) with the sample absorption.

Test signal: This is for testing the spectrometer.

LD (when LD accessory is installed): Linear dichroism signal, which is given by  $\sim AC/DC$  with 100 kHz.

ORD-M (when ORD-M accessory is installed): Optical rotational dispersion, which is given by  $\sim AC/DC$  with 100 kHz using an optical analyzer.

ORD-E (when ORD-E accessory is installed): Optical rotational dispersion which is controlled electronically.

UV (single): DC signal.

UV (single)-Abs: Converts the DC signal into the Abs value.

UV (double) (when UV (double) accessory is installed): Extends the double beam system to the short wavelength region.

FDCD (when FDCD accessory is installed): Fluorescence detected circular dichroism signal, which is also given by  $\sim AC/DC$  with 50kHz. Usually HT is fixed and DC varies. In this case, the AC component is displayed on Channel 1 (not FDCD).

FDCD/DC (when FDCD accessory is installed): Calculates the real FDCD value FDCD/DC.

[Channel #2] Selectable range: HT: Photomultiplier tube voltage, DC: Photomultiplier tube DC voltage, and Abs: calculated absorption value using the HT value.

[Channel #3] For external input signals (from the "EXT 1" terminal on the rear panel of

	the amplifier) and Abs.
[Channel #4]	For external input signals (from the "EXT 2" terminal on the rear panel of the amplifier).
Parameters	
[Sensitivity]	Selects the sensitivity from the drop-down list. Low            Up to 1000 mdeg Standard      Up to 200 mdeg High            Up to 5 mdeg
[D.I.T.]	Digital integration time per data. When the scan mode is set to [Step (Auto Response)], designate a range (in this case, the effective value extends to msec order).
[Band Width]	Sets the spectrum band width. Range: 0.01 nm – 15 nm, which is can be specified to two decimal places.
[Slit Width]	Sets the slit width. Can be entered by inserting a check mark in [Slit Width]. Range: 30 $\mu$ m to 3000 $\mu$ m (integer values only).
[Start]	Measurement start wavelength (long wavelength end). Range: 163 nm – 1100 nm.
[End]	Measurement end wavelength (short wavelength end). Range: 163 nm – 1100 nm.
[Data Pitch]	Selects the data acquisition interval from the drop-down list. Effective value extends to ms order.
[Start Mode]	This depends on the external trigger, which is intrinsic to an accessory. Immediate:            Performs a measurement without an external trigger. Wait for trigger:      Sets whether measurement is to be started by an external trigger or not (when stopped flow unit is installed).
[Scanning Mode]	Selects continuous scan or step scan as the scanning mode. Continuous mode: Performs “continuous scanning”. Step mode: Performs “step scanning”. Step (Auto Response) mode: Performs “step scanning” in which the DIT is variable.
[Scanning Speed]	Selects a wavelength scanning speed. Can be entered when the scan mode is set to [Continuous].
Accumulation/Repeat	
[Accumulation]	Sets the number of the accumulations for a measurement. Can be entered by inserting a check mark. Range: 1 – 999 times.
[Cycle Times]	Sets the number of measurements, which defines the number of the spectra acquired. Can be entered by inserting a check mark when [Accumulation] is off. Range: 1 – 999 times.
[Cycle Interval]	Sets the time between measurements. This is displayed when a number is

entered in the [Cycle Times] box. Range: 0 – 15000 sec.

- <OK> Transfers the set parameters to the spectrometer and closes the dialog box.
- <Cancel> Quits setting the parameters and closes the dialog box. Reverts to the previously defined parameters.
- <Open...> Loads the setting parameters from the disk.  
Clicking this button displays the [Open] dialog box. Selecting a baseline data file and clicking the <Open> button loads the baseline data into the memory. The data is in a .cdsp format file.
- <Save> Saves the parameters in a .cdsp format file.
- <Default> Reverts to the default parameters.

**CAUTION:** If the slit width is set manually, be careful not to set it too wide. If the slit width is too large the detector may be damaged. Do not set the HT voltage (photomultiplier voltage) to below 170 V.

**Note (1):** *If an inappropriate value is entered in [D.I.T.], [Data Pitch.], and [Scanning Speed] dialogs, an error message will be displayed.*

**Note (2):** *If the entered value exceeds the limits for that parameter, an error message will be displayed.*

**Note (3):** *The acceptable range of values for the [Band Width], [Start], and [End] is not the same as those for the instrument. Refer to “J-815 hardware manual” for its specification.*

**Note (4):** *Refer to “Appendix” for more information about parameters and suggestions on how to select them.*

**Note (5):** *The external input signal is acquired through the "EXT 1" and "EXT 2" terminals on the rear panel of the amplifier. The input range is -1 to +1 V. The output signal (DCV) can be acquired from an external device such as a thermostatted cell holder or a pH meter.*

### 3.1.1.2 [Control] Dialog Box

Turns [Baseline] correction ON/OFF and auto shutter driving. If baseline correction is turned on, the [Baseline] data will be subtracted from the sample spectra .

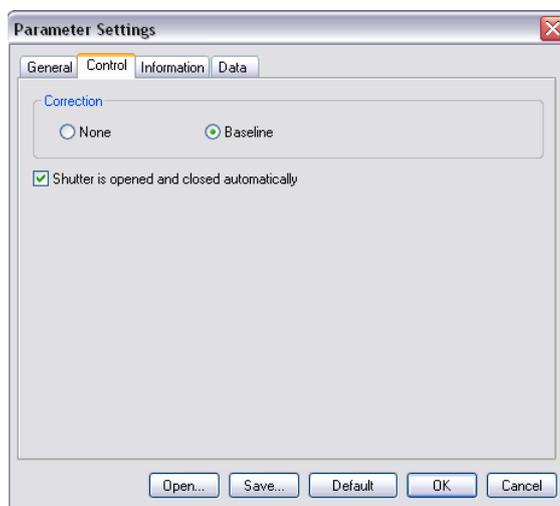


Figure. 3.3 [Control] dialog box

[Baseline] Turns the [Baseline] term ON, which results in a spectra measurement where the horizontal axis is time.

[None] Turns the correction OFF.

[Auto shutter is opened and closed automatically] Automatically opens the shutter just before measurement starts. Insert a check mark in this box if this function is required.

<OK> Transfers the set parameters to the spectrometer and closes the dialog box.

<Cancel> Quits setting and closes the dialog box. Reverts to the previously defined parameters.

<Open...> Baseline ON/OFF setting is loaded into the memory. Clicking this button displays the [Open] dialog box. Designating baseline data here and clicking the <Open> button loads the baseline data into the memory. The data is in a .cdsp format file.

<Save> Saves the baseline data. Saves the parameters defined in the [Parameter Setting] dialog box to disk. The data is saved as a .cdsp format file.

<Default> Reverts to the default parameters.

**Note:** *If baseline correction is carried out, the resulting spectra have had the baseline subtracted from them.*

The menus for which baseline correction is available are listed below.

Menu	Baseline correction
CD	Available
CD/DC	Not available
LD	Available
ORD-E	Available
ORD-M	Available
UV (single)	Available
UV(single)-Abs	Available
UV (double)	Available
FDCD	Available
FDCD/DC	Not Available
LB	Available
CB	Available
Fluorescence	Available
Test signal	Not Available

The “available correction” is indicated in the monitor bar of the [Spectra Measurement] window: if available, the corresponding value is displayed in white after baseline measurement has been performed.

### 3.1.1.3 [Information] Dialog Box

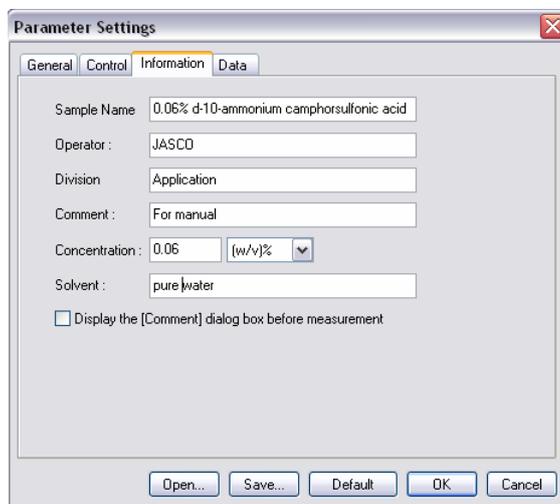


Figure. 3.4 [Information] dialog box

Set [Sample Name] (63), [Operator] (63), [Division] (110), [Comment] (126), [Solvent] (126), [Operator] (30), [Organization] (94) and [Comment] (126). The numbers in parentheses are the maximum numbers of characters that can be entered. The concentration units, mol/l, mmol/l,  $\mu$ mol/l, nmol/l, w/v%, ppm, and ppb, can be selected.

### 3.1.1.4 [Data] Dialog Box

Sets automatic saving, transferring to Spectra Analysis, and printing out of the spectra.

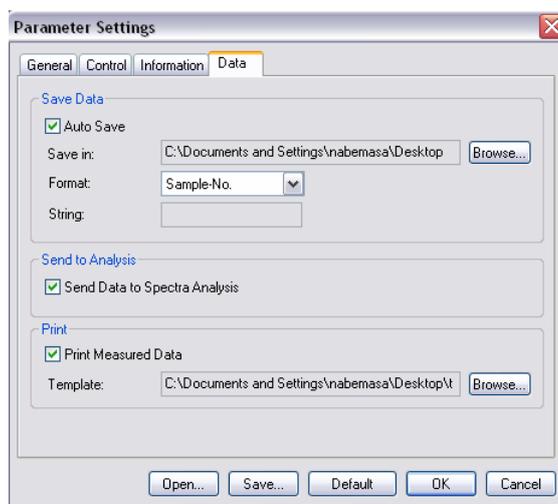


Figure. 3.5 [Data] dialog box

[Save Data]	Sets whether the acquired spectrum is to be saved automatically or not. If a check mark is put in the [Auto Save] box, enter a filename and directory in the dialog box. This is useful for the repeated measurements.										
[Save in]	Enter the file and directory name. The <Browse...> button is useful for selecting the directory.										
[Format]	<table border="0" style="width: 100%;"> <tr> <td style="padding-right: 20px;">Date-No.</td> <td>Displays the date and file number</td> </tr> <tr> <td>Sample-No.</td> <td>Displays the sample name and file number, 1, 2, 3...</td> </tr> <tr> <td>Comment-No.</td> <td>Display comments written in the [information] dialog box and the file number, 1, 2, 3...</td> </tr> <tr> <td>Sample-Comment-No:</td> <td>Displays Sample name and comment written in the [information] dialog box and the file number, 1, 2, 3...</td> </tr> <tr> <td>String-No.</td> <td>Displays the filename given in the [String:] box and the file number, 1, 2, 3...</td> </tr> </table>	Date-No.	Displays the date and file number	Sample-No.	Displays the sample name and file number, 1, 2, 3...	Comment-No.	Display comments written in the [information] dialog box and the file number, 1, 2, 3...	Sample-Comment-No:	Displays Sample name and comment written in the [information] dialog box and the file number, 1, 2, 3...	String-No.	Displays the filename given in the [String:] box and the file number, 1, 2, 3...
Date-No.	Displays the date and file number										
Sample-No.	Displays the sample name and file number, 1, 2, 3...										
Comment-No.	Display comments written in the [information] dialog box and the file number, 1, 2, 3...										
Sample-Comment-No:	Displays Sample name and comment written in the [information] dialog box and the file number, 1, 2, 3...										
String-No.	Displays the filename given in the [String:] box and the file number, 1, 2, 3...										
[String]	Allows the desired filename to be chosen, which is displayed as "String-No".										
[Print]	Determines whether a file number is to be affixed or not. If a check mark is inserted in the [Print Measured Data] box, enter a filename and directory in the dialog box. This is useful for the repeated measurements.										
[Send data to Spectra Analysis]	Transfers data to the [Spectra Analysis] program automatically.										

**Note (1):** The printing out form must be set in the [JASCO Canvas] window.

**Note (2):** When using the [Send data to Spectra Analysis] mode with several cycle times, multiple sets of data are sent to the [Spectra Analysis] window.

## 3.2 [Control] Menu

### 3.2.1 [Select Accessory...]

Registers an optional accessory to be used.

**Note:** Optional accessories should be registered before starting measurement.

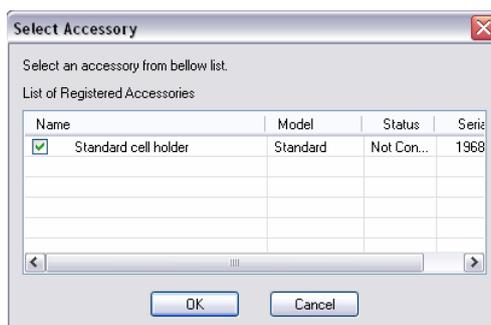


Figure. 3.6 [Select Accessories] dialog box

Insert a check mark in the box of the accessory name to be used. Standard cell holder is given as the default.

<OK> The selected optional accessory is registered and returns to the previous window.

<Cancel> Quits registration and closes the dialog box. Reverts to previous window.

**CAUTION:** Before using an electromagnet, remove the emission detector cable from the "DA1" connector on the rear panel of the spectrometer. Otherwise, a high voltage will be applied to the emission detector and may damage it.

### 3.2.2 [Move Wavelength...]

Moves the wavelength to the desired value.

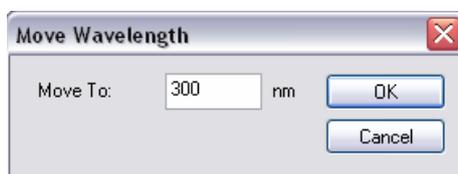


Figure. 3.7 [Move Wavelength] dialog box

[Wavelength] Text box for input. Range: 165 to 1100 nm.

<OK> Moves the wavelength to the selected wavelength.

<Cancel> Closes the dialog box without modifying the previous wavelength setting.

### 3.2.3 [CD Detector...]

Sets the detector (CD/ORD/LD/UV) sensitivity.

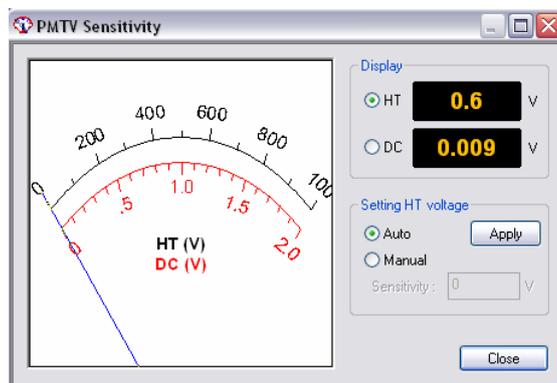


Figure. 3.8 [PMTV Sensitivity] dialog box

[Display] Changes over the meter indication (displayed to the right side of Fig. 3.8) at the right to [HT] or [DC] with an option button.

[HT] Displays the photomultiplier HT voltage.

[DC] Displays the photomultiplier DC voltage.

[Setting HT voltage] Select the [Auto] or [Manual] option button. If [Manual] is selected, input [Sensitivity] and click the <Apply> button. Set range: 0 to 1000 V

**CAUTION:** Set the HT voltage so that the DC voltage does not exceed 2 V. Otherwise, the detector may be damaged.

**Note:** Ensure that the menu of channel 2, which is set in the [Parameter Settings] dialog box, is set to DC. If it is not set to DC, the data will not be displayed in the [Spectra Measurement] window and will not be saved.

<Close> Transfers the set values to the spectrometer and closes the dialog box.

### 3.2.4 [Light Source...]

Turns the light source ON/OFF and displays the light source operating time.



Figure. 3.9 [Light Source Control] dialog box

[Xe Lamp] Turns the light source ON/OFF. The “light cube” icon can be toggled by clicking it.

 Indicates light source is ON.



Indicates light source is OFF.

The operating time of the lamp is displayed in Fig. 4.9 (for example, 0.0 hour)

<OK>

Turns the lamp on.

<Cancel>

Closes the dialog box without changing anything.

*Note: If the light source does not turn on, try turning it on several times. If it still does not come on contact your nearest JASCO office.*

### 3.2.5 [Shutter...]

Opens or closes the shutter. Effective for an spectrometer having a shutter.

This instrument uses a high output xenon lamp as the light source. It irradiates a sample with high intensity ultraviolet rays. When measuring a sample that is vulnerable to photolysis, minimize the irradiating time or narrow the slit width to reduce the beam intensity. In such a case, only open the shutter during measurements using this function.



Figure. 3.10 [Shutter Control] dialog box

[Shutter]

Turn the shutter ON/OFF. The icon of shutter can be toggled by clicking it.



Indicates shutter is open.

Indicates shutter is closed.

<OK>

Opens or closes the shutter.

<Cancel>

Closes the dialog box without changing anything.

*Note: Closing the shutters zeroes the HT voltage. Ensure that this is the case by checking the [CD Detector...] dialog box (Fig. 3.8) if necessary.*

*Note: When the spectrometer is turned ON, the shutter is open. Check that the front LED lamp for shutter ON/OFF is lit in this case.*

### 3.2.6 [ORD-M Zero Clear]

Effective when ORD-M is installed.

## 4. Practical Use of Spectra Measurement Program

This section explains the procedures for measuring a standard sample using the Spectra Measurement program, saving the measured spectrum to disk and printing it out.

### 4.1 Operation Overview of Spectra Measurement Program

Starting spectrometer	See "4.2.1"
↓	
Checking the Registration of Accessories	See "4.2.2".
↓	
Sample preparation	See "4.3.1".
↓	
Starting Spectra Measurement Program	See "4.3.2".
↓	
Setting Parameters	See "4.3.3".
↓	
Setting Sample	See "4.3.4".
↓	
Measuring Sample	See "4.3.4".
↓	
Saving Sample Spectrum, Baseline, and Parameters	See "4.3.5".
↓	
Sending Spectrum to Spectra Analysis	See "4.3.6".
↓	
Printing Spectrum	See "4.3.7".

### 4.2 Starting Spectrometer and Spectra Manager

#### 4.2.1 Starting Spectrometer

*Note: Refer to "2.1" and "2.2" for the starting up and turning off the spectrometer, respectively. Here, the explanation begins with starting up the measurement program from the [Spectra Manager] window.*

#### 4.2.2 Checking the Registration of Accessories

*Note: Refer to "2.4.4.1" for the registration of optional accessories, which is recommended.*

### 4.3 Measuring, Saving and Printing Spectra

The procedure for acquiring the spectrum of *d*-10-ammonium camphor sulfonic acid (NH<sub>4</sub>-CSA), which is a standard sample, saving the measured spectrum to disk and printing it out is described in this section.

#### 4.3.1 Sample Preparation

The sample used was 0.06% (w/v) *d*-10-ammonium camphorsulfonic acid (NH<sub>4</sub>-CSA) in an aqueous solution. Prepare a sample using NH<sub>4</sub>-CSA, which is a standard sample. Put the prepared sample into a 10 mm cell.

#### 4.3.2 Starting the Spectra Measurement Program

Double clicking the [Spectra Measurement] menu of [Spectra Manager] starts the Spectra Measurement program and the following window appears.

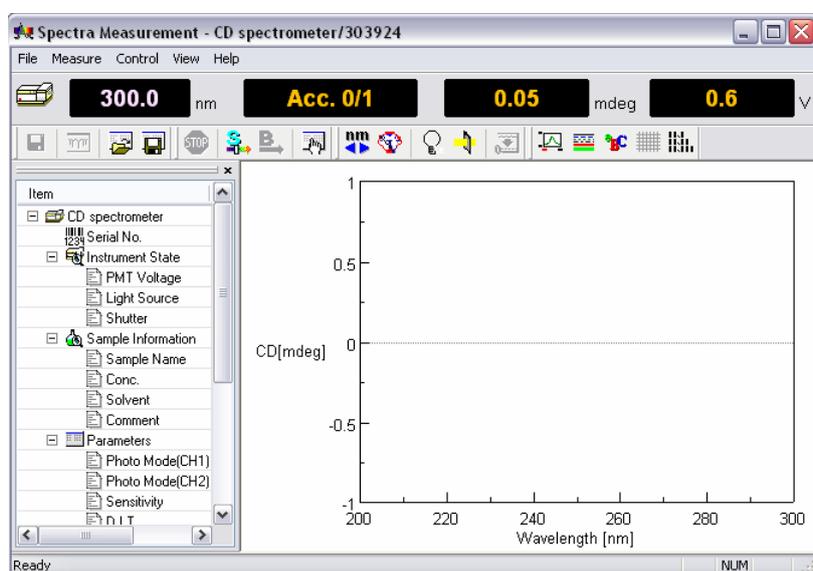


Figure. 4.1 [Spectra Measurement] window

### 4.3.3 Setting Parameters

- (1) Click  or select [Parameter] from [Measure] menu.

The following dialog box appears. The parameters setting dialog box is made up of the dialog boxes: [General], [Control], [Information] and [Data]. Clicking a top tab of the dialog box changes the dialog box (Refer to “3.1.1” for these functions and their descriptions).

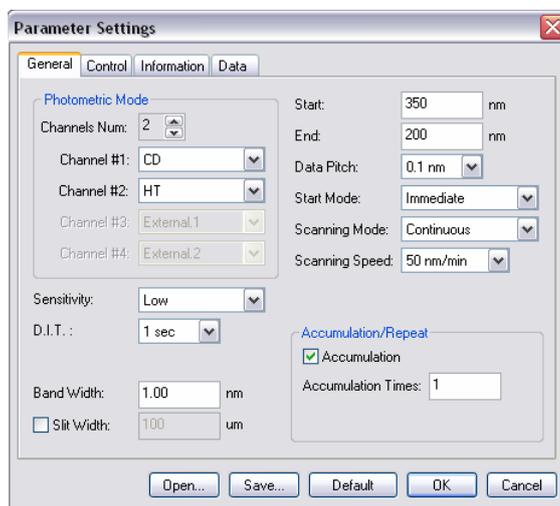


Figure. 4.2 [Parameter Settings] dialog box

- (2) Changing parameters in the [General] dialog box

Parameters currently displayed in the [Parameters] dialog box are selected. This is commonly used for checking CD accuracy using *d*-10-ammonium camphorsulfonic acid (NH<sub>4</sub>-CSA) in a pure water solution. Here, set them as follows (refer to “3.1.1.1” for a description of and the limits for the following parameters).

[Sensitivity]	Low
[Start Mode]	Immediate
[Start]	350 nm
[End]	200 nm
[Scanning Mode]	[Continuous]
[Scanning Speed]	50 nm/min
[Band Width]	1.0 nm
[D.I.T.]	1 sec
[Data Pitch]	0.1 nm
[Accumulation Times]	1

**Note (1):** The wavelength range and the number of accumulations are different from those given in the [Validation Program]. But this difference is not important for just checking the CD value.

**Note (2):** Refer to “Appendix” for setting appropriate values for [Scanning Speed] and the relationship between [D.I.T.], the S/N ratio and [Accumulation Times].

**Note (3):** Refer to “3.1.1.1” and “3.1.1.2”-“3.1.1.4” for more information regarding the following menus 1)-9) and 10), respectively.

- 1) Set [Sensitivity]  
[Sensitivity] is a drop-down box. Clicking the arrow on the extreme right displays a list of the sensitivities. Usually, [Standard] mode is employed, which is effective up to  $\pm 200$  mdeg. For measuring small CD values, the [Low] mode is the most effective. On the other hand, for large CD values, greater than  $\pm 200$  mdeg, the [High] mode should be employed.
- 2) Set [Start Mode]  
[Start Mode] is a drop-down box. Clicking the arrow on the extreme right displays a list of the [Start Mode]. If the external trigger is not required such is the case when using stopped flow accessories, use the [Immediate] mode.
- 3) Set [Start] and [End].  
Enter the upper wavelength into the [Start] text box, and the lower wavelength into the [End] text box. To input the value in [Start], for example, click its text box. A cursor appears in the text box, waiting for input. Delete unnecessary numerals and input a wavelength using the numeric keys.
- 4) Set [Scan Mode].  
[Scan Mode] is a drop-down box. Clicking the arrow on the extreme right displays a list of the [Scan Mode]. Almost all measurements can be performed in [Continuous] mode. In rare cases, gas phase CD measurements for example, “step scanning” should be employed. When selecting [Step (Auto Response)], the limits for the [D.I.T.] value must be set (see Setting [D.I.T.]).
- 5) Set [Scan Speed].  
[Scan Speed] is a drop-down box. Clicking the arrow on the extreme right displays a list of the [Scan Speed].
- 6) Set [Band Width].  
Input the half-width value in the [Band Width] text box.
- 7) Set [D.I.T.].  
[D.I.T.] is a drop-down box. Clicking the arrow on the extreme right displays a list of the [D.I.T.]. This is restricted by the [Scanning Speed] and by the [Band Width]. Supposing that the [Scanning Speed] and the [Band Width] have the values given in Fig. 4.2, for example. In this case, a single scan takes 1.2 sec/nm. So a band width of 1.0 nm is reasonable if the [D.I.T.] is set to be 1 sec or less. But a [D.I.T.] of over 1.2 sec is often preferred because the liquid phase broadens the CD spectrum considerably. An appropriate [D.I.T.] value should be selected by considering such broadening with the specified [Scanning Speed] and [Band Width].
- 8) Set [Data Pitch].  
[Data Pitch] is a drop-down box. Clicking the arrow on the extreme right displays a list of the sensitivities.
- 9) Set [Accumulation Times].  
Input the accumulation time in the [Accumulation Times] text box. The cycle time can also be specified.

- 10) Set the [Control] parameters and the values of [Information] and [Data].  
Enter the appropriate settings in the [Control], [Information] and [Data] dialog boxes.
- (3) On completion of setting parameters, clicking the <OK> button will transfer the parameters to the spectrometer. The transfer process is indicated by messages displayed on the screen. Check the parameters that appear in the window. Refer from “3.1.1.1” to “3.1.1.4” for usage of <Open...>, <Save...>, <Default>, and <Cancel>.
- (4) For the case when it is desired to use the same parameters used previously click the  button or select [Open Parameters...] in the [File] menu. The parameters are loaded into the window.

#### 4.3.4 Setting Sample and Measurement

- (1) Setting sample
  - 1) Set the cell holder on the cell holder receiver in the sample compartment so that the cell holder is in contact with the light shield.
  - 2) Put the cell in the left corner of the cell holder and lightly hold it with the cell holder facing down.

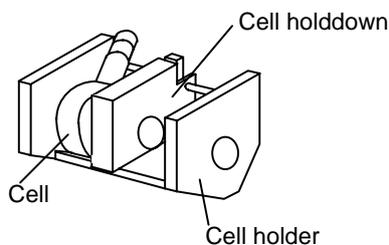


Figure. 4.3 Setting the cell

**Note:** Refer to “CD/ORD measuring method” for cell types.

- (2) Measurement
  - 1) Baseline measurement  
Clicking the [Baseline] from the [Measure] menu (or the  button) displays the following message dialog box.

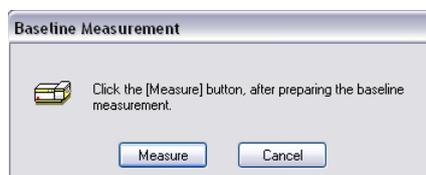


Figure. 4.4 Message box for starting [Baseline] measurement

Click <Measure> and the sample spectrum is acquired and the progress of measurement is displayed on the screen. If <Cancel> is clicked, the baseline measurement is interrupted the system waits for further instructions. Upon completion of measurement, the “Ready” comment appears on the [Status Bar] in the [Spectra Measurement] window. If an optional accessory is not registered in the [Select Accessory] - [Control] in the [Spectra Measurement] window, the following message appears.



Figure. 4.5 Message box for accessory

Click the <OK> button, and the sample is measured. If the <Cancel> button is clicked, the baseline measurement is interrupted and the system waits for further instructions. In the latter case, the accessory can be registered. Refer to “2.4.4.1” and “3.2.1” regarding registration of accessories. When it is necessary to abort the measurement completely, click  or select [Cancel] in the [Measure] menu.

**Note:** Suspending baseline CD measurement displays the spectrum acquired from [Start] up to the wavelength reached when the measurement was interrupted. When interrupted, the acquired data can not be used as a baseline spectrum.

When [Cycle Times] is selected, the baseline is given as follows.

**Note :** The baseline data is only a single spectrum. Even if several cycles are selected in the [Cycle times], the baseline correction is performed using a single baseline spectrum.

## 2) Sample measurement

Click [Sample] from the [Measure] menu (or the  button) after performing baseline measurement. If an optional accessory is not registered in [Select Accessory] - [Control] in the [Spectra Measurement] window, the dialog box of Fig. 4.5 appears. Upon completion of measurement, the “Ready” comment appears on the [Status Bar] in the [Spectra Measurement] window. Note the following cases.

CASE A: If the parameters are different between the sample and baseline measurements, the following dialog box is displayed.

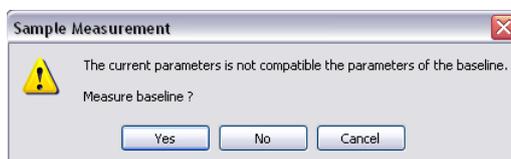


Figure. 4.6 Message box for sample measurement

Click <Yes>, and the baseline measurement is carried out using the current parameters. Click <No>, and the baseline measurement is carried out using the modified measurement conditions. Click <Cancel>, and the baseline measurement is interrupted and the system waits for next instruction. When it is necessary to abort the measurement click the  button or select [Cancel] in the [Measure] menu.

CASE B: If baseline measurement was not performed, the sample is measured without baseline correction.

**Note (1):** Suspending baseline CD measurement displays the spectrum acquired from [Start] up to the wavelength reached when the measurement was interrupted. This is also the same with the case when [Cycle Times] is selected.

**Note (2):** Baseline measurement should be completed when it is desired to acquire baseline corrected sample spectra.

**Note (3):** The same measurement parameters should be employed for both the sample and baseline measurements.

### 4.3.5 Saving Spectra

**Note :** Refer also to Section 3.1.1.

#### 4.3.5.1 Saving Parameters

Saves parameters to disk.

**Note :** Save parameters when the parameter setting is activated.

(1) Click [Save Parameters...] from the [File] menu, which is on the [Spectra Measurement] screen. The same operation can be performed by clicking the  button. The following dialog box appears.

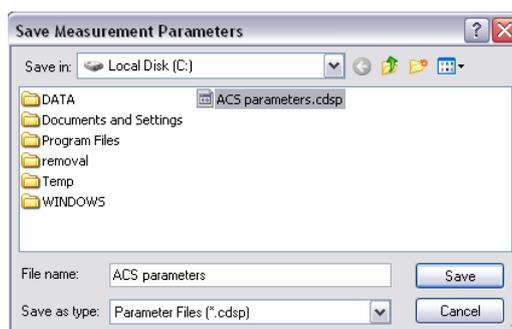


Figure. 4.7 [Save parameters] dialog box

- (2) Select a location to save the spectrum by clicking the arrow on the extreme right in the [Save in] box (in Fig. 4.7, “Local Disk (C)” is selected).
- (3) Input a filename in the [File Name] text box. The extension (after “.”) need not be entered. The output file is saved as a .cdsp format file.
- (4) Click the <Save> button, and the spectrum is saved to disk (the file name in Fig. 4.7 is “ACS parameters”)

#### 4.3.5.2 Saving Baseline Data

Saves a baseline spectrum to disk.

**Note :** *Save it when the baseline measurement is completed.*

- (1) Click [Save Baseline...] from the [File] menu, which is on the [Spectra Measurement] screen. The following dialog box appears.



Figure. 4.8 [Save baseline] dialog box

**Note:** *The [Save Baseline...] is available after baseline measurement are completed or the baseline data is loaded onto the [Spectra Measurement].*

- (2) Select a location to save the spectrum by clicking the arrow on the extreme right in the [Save in] box (in Fig. 4.7, “Local Disk (C)” is selected).
- (3) Input a filename into the [File Name] text box. The extension (after ".") need not be entered. The output file is saved as a .cdbsl format file.
- (4) Click the <Save> button, and the spectrum is saved to disk (the file name of Fig. 4.8 is “water\_base”).

**Note:** *The baseline data is only a single spectrum. Even if several cycles are selected in the [Cycle times], the baseline correction for sample measurement is performed using a single baseline spectrum.*

### 4.3.5.3 Saving Sample Data

Saves a measured sample spectrum to disk.

**Note :** *Save sample data when sample measurement has been completed.*

- (1) Click [Save Data...] from the [File] menu, which is on the [Spectra Measurement] screen. The same operation can be performed by clicking the  button. The following dialog box appears.

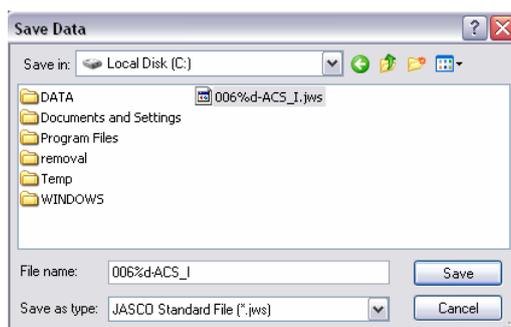


Figure. 4.9 [Save data] dialog box

**Note :** *The [Save data] is available after sample measurement is completed or sample data is loaded onto the [Spectra Measurement].*

- (2) Select a location to save the spectrum clicking the arrow at extreme right in the [Save in] box (in Fig. 4.7, “Local Disk (C)” is selected).
- (3) Input a filename in the [File Name] text box. The extension (after ".") need not be entered. The output file is saved as a .jws format file.
- (4) Clicking the <OK> button saves the spectrum to disk (the filename of Fig. 4.7 is “0.06%d-ACS\_I”).
- (5) In the case when, for example, “Cycle Times” is set to three, three sets of data are saved as xxx\_01.jws, xxx\_02.jws, and xxx\_03.jws.

**Note :** *Suspending measurement displays the spectrum acquired from [Start] up to the wavelength reached when the measurement was interrupted. This is also the same with the case when [Cycle Times] is selected.*

### 4.3.6 Transferring a Spectrum to [Spectra Analysis]

Transfers a measured spectrum to the [Spectra Analysis] window.

- (1) Click [Analysis Send] from the [File] menu or click  in the [Spectra Measurement] window. The [Spectra Analysis] window is automatically opened.
- (2) When [Cycle Times] is selected, the following dialog box appears after clicking [Analysis Send] (in Fig. 4.10, Cycle Times is set to 3).

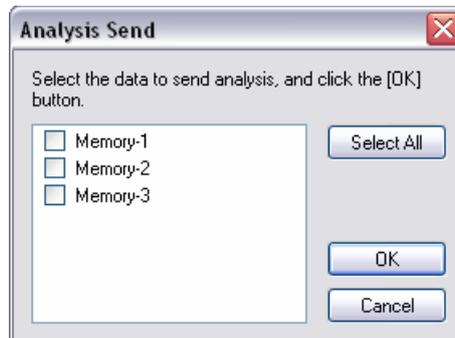


Figure. 4.10 [Save As...] dialog box

- (3) Insert checkmarks in the boxes of Fig. 4.10 and click the <OK> button. The selected data are transferred to [Spectra Analysis]. All the data can be transferred to [Spectra Analysis] by clicking <Select All>.

**Note :** If sample data is not saved (see [Save Data]), a filename is automatically assigned such as “Memory”. For the case [Cycle time] when is specified, the filenames are assigned as “Memory-1”, “Memory-2”, “Memory-3”... (see Fig.4.10). When sample data is saved, the filename can be renamed.

### 4.3.7 Printing Spectrum

Printing out the measured spectrum can be performed in the [Spectra Analysis] window. Click [Print...] from the [File] menu, and the spectrum is printed out. [Print Setup...] is useful when an output title is needed.

**Note :** Refer to “Spectra Analysis manual” for more details.

## 5. [Time Course Measurement] Menu Reference

Starting the Spectra Measurement program displays the following window.

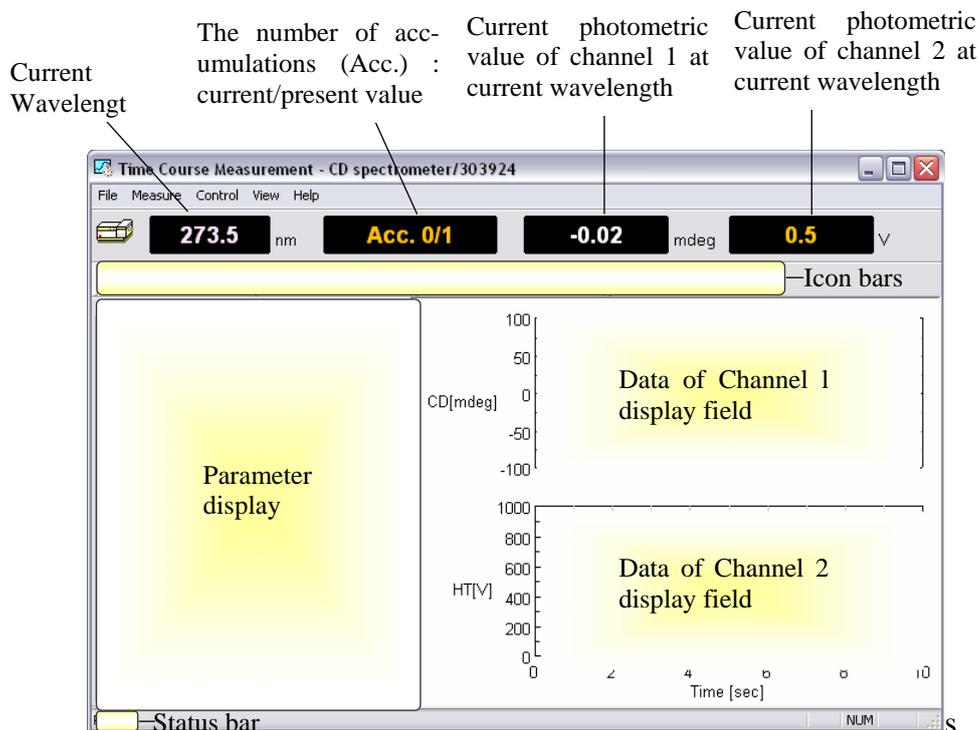


Figure. 5.1 [Time Course Measurement] window

**Note:** The program can display up to four types of data simultaneously by changing the number of measuring channels.

### [File] menu

- |                      |  |
|----------------------|--|
| [Save Data...]       | Saves the experimental data, measurement parameters, and set terms in a .jws format file.                                |
| [Analysis Send]      | Transfers the experimental data to the [Spectra Analysis] window, which starts automatically when using [Analysis Send]. |
| [Open Parameters...] | Opens parameters which is set in the [Parameter Settings] dialog box. The file is saved in .cdsp format.                 |
| [Save Parameters...] | Save parameters in a .cdsp format file.  |
| [Exit]               | Exits the [Spectra Measurement] window.  |

### [Measure] menu

- |                 |  |
|-----------------|--|
| [Parameters...] | Sets parameters, turns the baseline measurement ON/OFF and auto-shutter drive, edits comments and saves and loads measurement parameters and data onto or from the disk. |
| [Sample]        | Starts measurement of sample.  |
| [Baseline]      | Starts [blank] and [baseline] measurement and turns these OFF.   |
| [Cancel]        | Stops baseline and sample measurement.   |

## [Control] menu

[Move Wavelength...]	Moves the current wavelength to the desired value.
[CD Detector...]	Sets the detector (CD/ORD/LD/UV) sensitivity.
[Light Source...]	Turns the light source ON/OFF. Displays/initializes the light source operating time.
[Shutter...]	Opens or closes the shutter (when installed).
[Auto Zero]	Zeroes the photometric value of ORD-M (when installed).
[Accessory...]	Registers compatible accessories.

## [View] menu

[Select Graph...]	Selects the desired channel No. (default is channel 1).
[Overlay]	Overlays the graphs.
[Scale...]	Sets the minimum and maximum values for the vertical and/or horizontal axes/axis.
[Pattern...]	Selects the color of CD curve, HT curve, etc.
[Font...]	Sets the font type of axes values and/or unit(s).
[Grid...]	Displays or hides grid.
[Style...]	Sets the scale interval.
[Select Graph...]	Selects which graphs are displayed or hidden.
[Information Bar]	Displays or hides parameter such as those shown in Fig. 4.1.
[Toolbar...]	Displays or hides the toolbars shown in Fig. 4.1.
[File]	Displays or hides the toolbar  .
[Measure]	Displays or hides the toolbar  .
[Control]	Displays or hides the toolbar  .
[View]	Displays or hides the toolbar  .
[Status Bar...]	Displays or hides the status bar of Fig. 4.1.
[Customize Toolbar...]	Selects the icons to be displayed and defines the appearance of the toolbar.

## [Help] menu

[Contents]	Displays the contents of the instrument.
[About...]	Displays the version and copyright.

## 5.1 [Measurement] Menu

### 5.1.1 [Parameters...]

Sets parameters, turns shutter ON/OFF for [blank] and [baseline] measurements and auto-shutter drive, edits comments and saves and loads measurement parameters and data onto or from disk. The parameters dialog box is made up of four dialog boxes: [General], [Control], [Information] and [Data]. They can be changed by clicking the appropriate tab at the top of the box. Clicking the tab [Data], for example, when the [Parameters Settings] dialog box is active displays the [Data] dialog box. The dialog boxes are described below.

#### 5.1.1.1 [General] Dialog Box

Sets the parameters of the spectrometer.

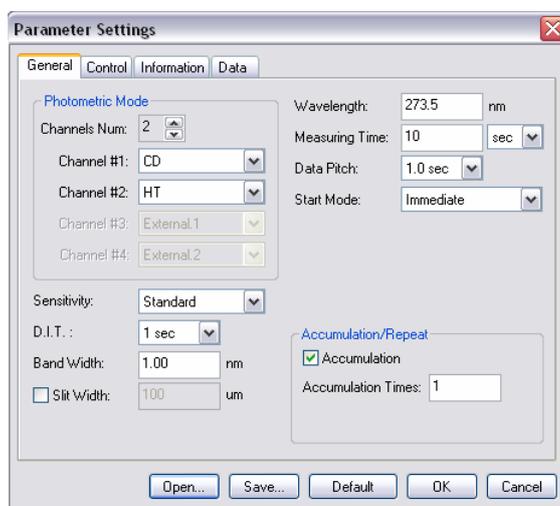


Figure. 5.2 [General] dialog box

#### Photometric mode

[Channel Num] Maximum of four channels. Four types of data can be acquired simultaneously.

[Channel #1] The selectable range varies with an optional accessory.

CD: Circular dichroism signal, which is given by  $\sim AC/DC$  with 50 kHz.

CD/DC: This is the same with CD mode when DC sets to 1 V. This mode is useful when the DC varies (i.e., HT is fixed at an arbitrary value) according to the sample absorption.

Test signal: This is for testing the spectrometer.

LD (when LD accessory is installed): Linear dichroism signal, which is given by  $\sim AC/DC$  with 100 kHz.

ORD-M (when ORD-M accessory is installed): Optical rotational dispersion, which is given by  $\sim AC/DC$  with 100 kHz using optical analyzer.

ORD-E (when ORD-E accessory is installed): Optical rotational dispersion, which is controlled electronically.

UV (single): DC signal.

UV (single)-Abs: Converts the DC signal into the Abs value.

UV (double) (when UV (double) accessory is installed): Extends the double beam system to the short wavelength region.

FDCD (when FDCD accessory is installed): Fluorescence detected circular dichroism signal, which is also given by  $\sim$ AC/DC with 50kHz. Usually HT is fixed and DC varies. In this case, the AC component is displayed on Channel 1 (not FDCD).

FDCD/DC (when FDCD accessory is installed): Calculates the real FDCD value FDCD/DC.

[Channel #2] Selectable range: HT: Photomultiplier tube voltage, DC: Photomultiplier tube DC voltage, and Abs: calculated absorption value using the HT value.

[Channel #3] For external input signals (from the "EXT 1" terminal on the rear panel of amplifier) and Abs.

[Channel #4] For external input signals (from the "EXT 2" terminal on the rear panel of amplifier).

#### Parameters

[Sensitivity] Selects sensitivity from the drop-down list.

Low Up to 1000 mdeg

Standard Up to 200 mdeg

High Up to 5 mdeg

[D.I.T.] Digital integration time per data. When the scan mode is set to [Step (Auto Response)], designate a range. This can be specified with an accuracy of 1 msec.

[Band Width] Sets the spectrum band width. Range: 0.01 – 15 nm, which can be specified to two decimal places.

[Slit Width] Sets the slit width. Can be entered by inserting a check mark in [Slit Width]. Range: 30  $\mu$ m to 3000  $\mu$ m (integer values only).

[Wavelength] Measurement wavelength range: 163 – 1100 nm, which can be specified to one decimal place.

[Measuring Time] Sets the measuring time, which is an integer. Select the units from the drop-down list. The value can be specified with an accuracy of 1 msec.

[Data Pitch] Selects the data acquisition interval from a drop-down list. This can be specified with an accuracy of 1 msec.

[Start Mode] This depends on the external trigger, which is intrinsic to an accessory.

Immediate: Runs measurement without external trigger.

Wait for trigger: Sets whether measurement is to be started by external trigger or not (when stopped flow unit is installed).

#### Accumulation/Repeat

[Accumulation] Sets the number of the accumulations for a measurement. Can be entered by inserting a check mark. Range: 1 – 999 times.

[Cycle Times] Sets the number of measurements, which defines the number of the spectra acquired. Can be entered by inserting a check mark when [Accumulation] is off. Range: 1 – 999 times.

[Cycle Interval] Sets the time between measurements. This is displayed when a number is entered in the [Cycle Times] box. Range: 0 – 15000 sec.

<OK> Transfers the set parameters to the spectrometer and closes the dialog box.

- <Cancel>                Quits setting the parameters and closes the dialog box. Reverts to the previously defined parameters.
- <Open...>              Loads the setting parameters from the disk.  
Clicking this button displays the [Open] dialog box. Selecting a baseline data here and clicking the <Open> button loads the baseline data into memory. The data is given as.cdtm format file.
- <Save>                    Saves the parameters in a .cdtm format file.
- <Default>                Reverts to the default parameters.

**CAUTION:** If the slit width is set manually, be careful not to set it too wide. If the slit width is too large the detector may be damaged. Do not set the HT voltage (photomultiplier voltage) to below 170 V.

*Note (1): If over-limitation value is remarked, the error message is displayed*

*Note (2): The over-accuracy values of [Band Width], [Slit Width], and [Wavelength] are ignored and acceptable values are shown on the comment and/or graph display field of Fig. 5.1.*

*Note (3): The external input signal is acquired through "EXT 1" and "EXT 2" terminals on the amplifier rear panel. The input range is -1 to +1 V. Output signal (DCV) can be acquired from an external device such as thermostatic cell holder or pH meter.*

### 5.1.1.2 [Control] Dialog Box

Terns ON/OFF [Baseline] or [Blank] correlation and auto shutter driving. If the correlation is turned on, sample spectra will be subtracted by the [Baseline] or [Blank] data.

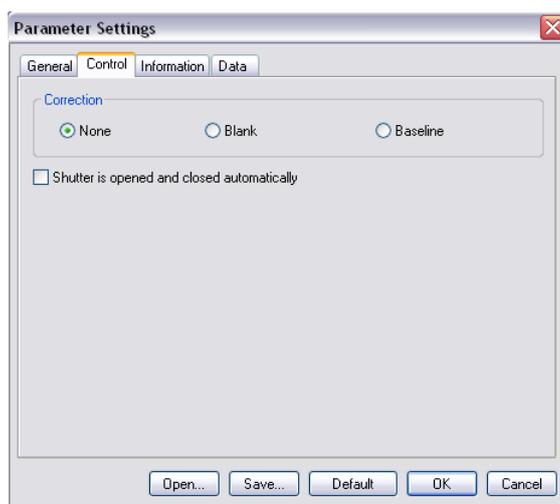


Figure. 5.3 [Control] dialog box

[Blank]                    Sets [Blank] term ON, which is “one-point” correlation given as  $[Blank]=[Accumulation] \times [D.I.T.]$ .

[Baseline]	Sets the [Baseline] term ON, which is a spectra measurement where the horizontal axis is time.
[None]	Turns the correction OFF.
[Auto shutter]	Automatically opens the shutter just before measurement starts. Puts the check mark if this function is necessary.
<OK>	Transfers the set parameters to the spectrometer and closes the dialog box.
<Cancel>	Quits setting and closes the dialog box. Control returns to previous parameters.
<Open...>	Baseline ON/OFF term is loaded into memory. Clicking this button displays the [Open] dialog box. Designating baseline data here and clicking the <Open> loads the baseline data into memory. The data exists as a.cdtm format file.
<Save>	Saves baseline data. Saves the parameters written in the [Parameter Setting] dialog box to disk. The data is memorized as a.cdtm format file.
<Default>	Sets the parameters default.

**Note (1):** *If baseline correction is carried out, the result is also subtracted one.*

**Note (2):** *The [Baseline] and [Blank] data cannot be saved.*

The menus that baseline correction is available are listed as follows.

<b>Menu</b>	<b>Baseline correction</b>
<b>CD</b>	Available
<b>CD/DC</b>	Not available
<b>LD</b>	Available
<b>ORD-E</b>	Available
<b>ORD-M</b>	Available
<b>UV (single)</b>	Available
<b>UV(single)-Abs</b>	Available
<b>UV (double)</b>	Available
<b>FDCD</b>	Available
<b>FDCD/DC</b>	Not Available
<b>LB</b>	Available
<b>CB</b>	Available
<b>Fluorescence</b>	Available
<b>Test signal</b>	Not Available

The “available correction” can be distinguished at the monitor bar in the [Spectra Measurement] window: if available, corresponding value is displayed in the “white color” after baseline measurement is achieved. (See channel #1 monitor bar of Fig. 5.1)

### 5.1.1.3 [Information] Dialog Box

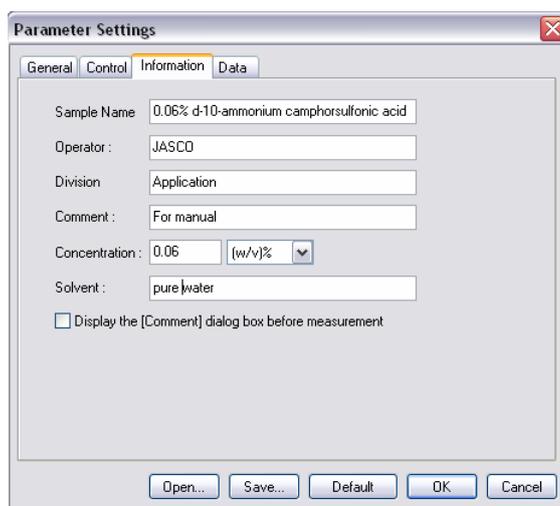


Figure. 5.4 [Information] dialog box

Set [Sample Name] (63), [Operator] (63), [Division] (110), [Comment] (126), [Solvent] (126), [Operator] (30), [Organization] (94) and [Comment] (126). The numbers in parentheses are the maximum numbers of characters. The concentration unit, mol/l, mmol/l,  $\mu$ mol/l, nmol/l, w/v%, ppm, and ppb can be selected.

### 5.1.1.4 [Data] Dialog Box

Sets automatic saving, transfers to Spectra Analysis, and Printing out the spectra.

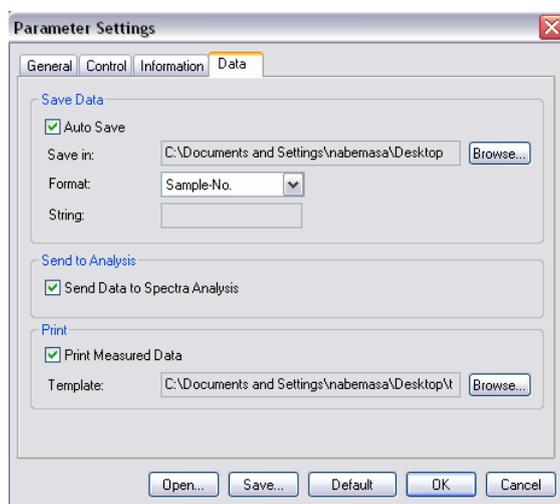


Figure. 5.5 [Data] dialog box

[Save Data]

Sets whether measured spectrum is to be saved automatically or not. If a check mark is put in the [Auto Save] box, enter a dialog box where a filename and directory are defined. This is useful for the repeatable measurement.

[Save in]

Puts the file and directory name. The <Browse...> button is useful for assigning the address.

[Format]

Date-No. Displays date and file number  
Sample-No. Displays sample name and file number, 1,

	2, 3...
Comment-No.	Displays comment written in the [information] dialog box and file number, 1, 2, 3...
	Sample-Comment-No Displays Sample name and comment written in the [information] dialog box and file number, 1, 2, 3...
String-No.	Displays the filename given in the [String] box and the file number, 1, 2, 3...
[String]	Puts the filename as you like, which is displayed as "String-No".
[Print]	Sets whether a file number is to be affixed or not. If a check mark is put in the [Print Measured Data] box, enter a dialog box where a filename and directory are defined. This is useful for the repeatable measurement.
[Send data to Spectra Analysis]	Sends data to the [Spectra Analysis] program automatically.

**Note (1):** *The printing out form must be set in the [JASCO Canvas] window.*

**Note (2):** *When using the [Send data to Spectrs Analysis] mode with several cycle times, the plural number of data is sent to the [Spectra Analysis] window.*

## 5.2 [Control] Menu

### 5.2.1 [Select Accessory...]

Resistors an optional accessory to be used.

**Note:** *Optional accessory should be registered before starting measurement.*

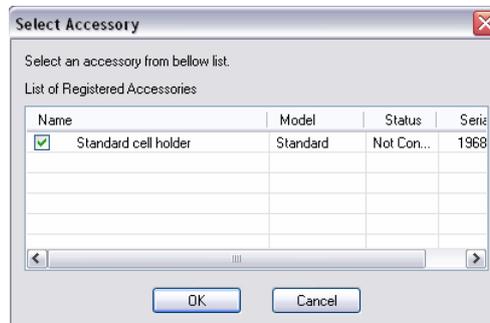


Figure. 5.6 [Select Accessories] dialog box

Puts the check mark in the box of the accessory name to be used. Standard call holder is given as default.

<OK> The selected optional accessory is registered and return to the previous window.

<Cancel> Quits the registration and closes the dialog box. Control returns to previous.

**CAUTION:** Before using an electromagnet, remove the emission detector cable from the "DA1" connector on the rear panel of the spectrometer. Otherwise, a high voltage will be applied to the emission detector and may damage it.

### 5.2.2 [Move Wavelength...]

Moves the wavelength to a desired value.



Figure. 5.7 [Move Wavelength] dialog box

[Wavelength] Text box for input. Range: 165 nm to 1100 nm.

<OK> Moves the wavelength to a set wavelength.

<Cancel> Closes the dialog box without changing previous wavelength setting.

### 5.2.3 [CD Detector...]

Sets detector (CD/ORD/LD/UV) sensitivity.

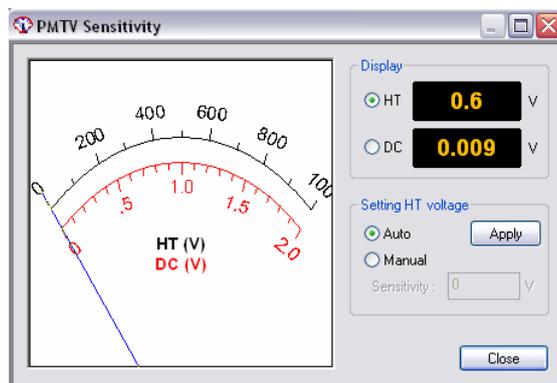


Figure. 5.8 [PMTV Sensitivity] dialog box

[Display] Changes over the meter indication (displayed to the right side of Fig. 5.8) at the right to [HT] or [DC] with an option button.

[HT] Displays the photomultiplier HT voltage.

[DC] Displays the photomultiplier DC voltage.

[Setting HT voltage] Select [Auto] or [Manual] with option button. If [Manual] is selected, input [Sensitivity] and click the <Apply> button. Set range: 0 to 1000 V

**CAUTION:** Set the HT voltage so that the DC voltage does not exceed 2 V. Otherwise, the detector may be deteriorated or damaged.

**Note:** Ensure that the menu of channel 2, which is set in the [Parameter Settings] dialog box, is DC. If it is not DC, the data is not displayed on the [Spectra Measurement] window and then cannot be obtained.

<Close> Transfers the set value to the spectrometer and closes the dialog box.

### 5.2.4 [Light Source...]

Turns ON/OFF the light source and displays the light source operating time.



Figure. 5.9 [Light Source Control] dialog box

[Xe Lamp] Turn ON/OFF the light source. The the “light cube” icon is changed alternatively by clicking it.



The sign turning on.



The sign turning off.

The operating time of light is displayed on Fig. 5.9. (0.0 hour, for example)

<OK>

Begins the lamp being lit.

<Cancel>

Closes the dialog box without changing anything.

*Note: If the light source is not lit, try it several times. If you have a trouble about it, contact your local JASCO distributor.*

### 5.2.5 [Shutter...]

Opens or closes the shutter. Effective for an instrument having a shutter.

This instrument uses a high output xenon lamp as the light source. It irradiates sample with high intensity ultraviolet rays. When measuring a sample that is vulnerable to photolysis, minimize the irradiating time or narrow the slit width to lower the beam intensity. In such a case, open the shutter only during measurement by using this function.



Figure. 5.10 [Shutter Control] dialog box

[Shutter]

Turn ON/OFF the shutter. The icon of shutter is changed alternatively by clicking it.



Shutter is open.

Shutter is closed.

<OK>

The shutter opens or closes.

<Cancel>

Closes the dialog box without changing anything.

*Note: Closing the shutters zeroes the HT voltage. Ensure it in the [CD Detector...] dialog box (Fig. 5.8) if necessary.*

*Note: When the spectrometer is turned ON, the shutter is open state. Check that the front LED lamp for shutter ON/OFF is lit in this case.*

### 5.2.6 [ORD-M Zero Clear]

Effective when ORD-M is installed.

## 6. Practical Use of Time Course Measurement Program

This section explains the procedure for, measuring a sample using Time Course Measurement program, saving the measured data to disk and printing it out for exercise in the operation of the spectrometer.

### 6.1 Operation Overview of Time Course Measurement Program

Starting Instrument	See "6.2.1"
↓	
Checking the Registration of Accessories	See "6.2.2".
↓	
Sample preparation	See "6.3.1".
↓	
Starting Time Course Measurement Program	See "6.3.2".
↓	
Setting Parameters	See "6.3.3".
↓	
Setting Sample	See "6.3.4".
↓	
Measuring Sample	See "6.3.4".
↓	
Saving Sample Data and Parameters	See "6.3.5".
↓	
Sending Data to Spectra Analysis	See "6.3.6".
↓	
Printing Spectrum	See "6.3.7".

## 6.2 Starting instrument and Spectra Manager

### 6.2.1 Starting Instrument

**Note:** Refer to "2.1" and "2.2" for the starting up and turning off the instrument, respectively. Here, explanation begins with startup of the measurement program from the [Spectra Manager] window.

### 6.2.2 Checking the Registration of Accessories

**Note:** Refer to "2.4.4.1" and "3.2.1" for the registration of optional accessories, which has been recommended these days.

## 6.3 Measuring, Saving and Printing Data

The procedure for measuring photo dissociation of *d*-10-ammonium camphorsulfonic acid (NH<sub>4</sub>-CSA) in water solution, for example, saving the measured spectrum onto a memory disk and printing it out is given here.

### 6.3.1 Sample Preparation

As sample is used 0.06% (w/v) *d*-10-ammonium camphorsulfonic acid (NH<sub>4</sub>-CSA) in water solution. Prepare a sample using NH<sub>4</sub>-CSA, which is a standard accessory. Put the prepared sample into a 0.2 mm cell, for example.

### 6.3.2 Starting the Time Course Measurement Program

Double click [Time Course Measurement] menu of [Spectra Manager]. The Time Course Measurement program starts and the following window appears.

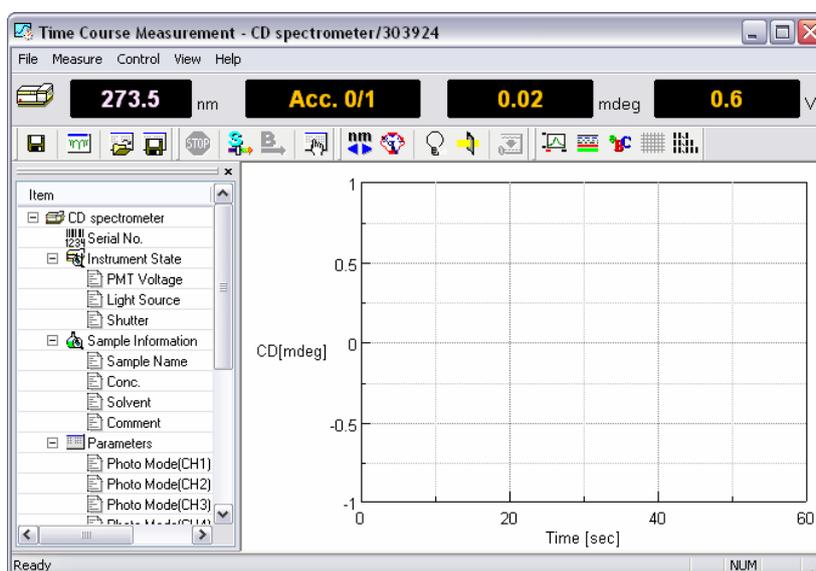


Figure. 6.1 [Spectra Measurement] window

### 6.3.3 Setting Parameters

- (1) Click  or select [Parameter] from [Measure] menu.

The following dialog box appears. The parameters setting dialog box is made up of dialog boxes: [General], [Control], [Information] and [Data]. Clicking a top tab changes over the dialog box. (Refer to “5.1.1” for these functions and meaning)

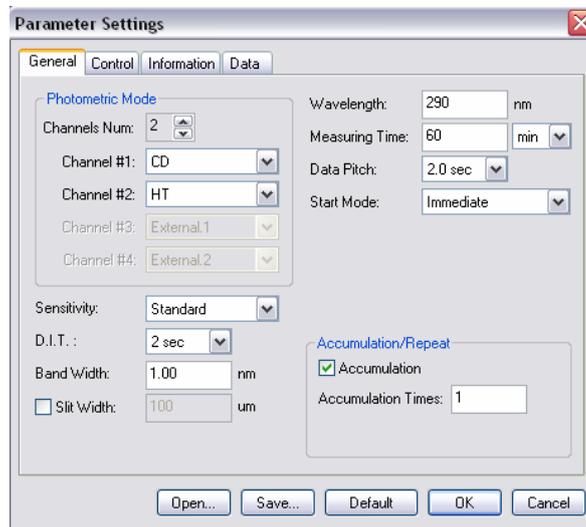


Figure. 6.2 [Parameter Settings] dialog box

- (2) Changing parameters in the [General] dialog box

Parameters currently displayed in the [Parameters] dialog box are selected. Set them, for example as follows. (Refer to “5.1.1.1” for the meaning of the following parameters)

[Sensitivity]	Standard
[Start Mode]	Immediate
[Wavelength]	290 nm
[Band Width]	1.0 nm
[Measuring Time]	60 min
[D.I.T.]	2 sec
[Data Pitch]	2.0 sec
[Accumulation Times]	1

**Note (1):** Refer to J-815 hardware manual for the hard wear limitation of wavelength and band width.

**Note (2):** Refer to “5.1.1.1” and “5.1.1.2”-“5.1.1.4” for more information regarding the following menus 1)-9) and 10), respectively.

- 1) Sets [Sensitivity]

[Sensitivity] is a drop-down type box. Click the arrow at extreme right. A list of sensitivities is displayed. Although [Low] is also available, [Standard] is rather appropriate because CD becomes smaller in accordance with the photo dissociation enhanced.

- 2) Sets [Start Mode]  
[Start Mode] is a drop-down type box. Click the arrow at extreme right. A list of sensitivities is displayed. If not needed the external trigger such as stopped flow accessories, the [Immediate] mode is employed.
- 3) Sets [Wavelength].  
Input desirable wavelength into the [Wavelength] text box. To input [Wavelength], for example, click its text box. A cursor appears in the text box, waiting for input. Delete unnecessary numerals and input a wavelength with numeric keys.
- 4) Sets [Band Width].  
Input the half-width value into the [Band Width] text box.
- 5) Sets [D.I.T.].  
[D.I.T.] is a drop-down type box. Click the arrow at extreme right. A list of sensitivities is displayed. This is just time and is different form that of [Continuous Scanning].
- 6) Sets [Data Pitch].  
[Data Pitch] is a drop-down type box. Click the arrow at extreme right. A list of sensitivities is displayed.
- 7) Sets [Accumulation Times].  
Input the accumulation times into the [Accumulation Times] text box. Cycle time is also available.
- 8) Sets parameters of [Control], terms of [Information] and [Data].  
Do appropriate setting in the [Control], [Information] and [Data] dialog box. Selects [Blank] or [Baseline] correction desirable.
- (3) Upon completion of parameter setting, click the <OK>. Parameters are transferred to the spectrometer. The transfer process is displayed by messages on the screen. Check parameters appeared on the window. Refer to “5.1.1.1”-“5.1.1.4” for usage of <Open...>, <Save...>, <Default>, and <Cancel>.
- (4) In the case the same parameters previously used is employed, click  or select [Open Parameters...] in the [File] menu. The parameters are loaded into the window.

### 6.3.4 Setting Sample and Measurement

(1) Setting sample

- 1) Set the cell holder on the cell holder receiver in the sample compartment so that the cell holder is in contact with the light shield.
- 2) Put the cell in the left corner of the cell holder and lightly hold it with the cell hold down.

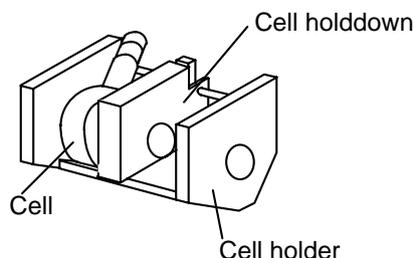


Figure. 6.3 Setting the cell

**Note (1):** Refer to "CD/ORD measuring method" for cell types.

**Note (2):** Refer to "Stopped Flow" manual when using SFA attachment.

(2) Measurement

1) Baseline measurement

Click [Baseline] from the [Measure] menu (or  button), and one of the following message dialog boxes is displayed.



Figure. 6.4 Message boxes for starting [Baseline] measurement

Click <Measure> and the sample is measured and the progress of measurement is displayed on the screen. If Clicking <Cancel>, baseline measurement is not carried out and waits for next instruction. Upon completion of measurement, the comment "ready" is displayed on the [Status Bar] in the [Spectra Measurement] window. If optional accessory is not registered in the [Select Accessory] - [Control] in the [Spectra Measurement] window, the following message appears.



Figure. 6.5 Message box for accessory

Click <OK>, and the sample is measured. But click <Cancel> and the baseline measurement is interrupted and waits for next instruction. In the latter case, the registration of accessory can be accessible. Refer to “2.4.4.1” and “5.2.1” about the registration. When the measurement has to do emergency stop, click  or select [Cancel] in the [Measure] menu.

**Note (1):** *The [Baseline] and [Blank] data cannot be saved.*

**Note (2):** *Suspending blank CD measurement displays a spectrum from [Start] to measured wavelength in the View. When interrupted, the data does not work as a baseline spectrum.*

In the case the [Cycle Times] is selected, the baseline is given as follows.

**Note (3):** *The baseline data, [Blank] or [Baseline] is only one data. Even if several numbers of cycles is selected in the [Cycle times], the baseline correction is performed using such baseline data.*

## 2) Sample measurement

Click [Sample] from the [Measure] menu (or  button) after baseline measurement. If optional accessory is not registered in the [Select Accessory] - [Control] in the [Time Course Measurement] window, the dialog box of Fig.6.5 appears. Upon completion of measurement, the comment “ready” is displayed on the [Status Bar] in the [Time Course Measurement] window. Note the following cases.

CASE A: If the parameters are different between sample and baseline measurement, the following dialog box is displayed.

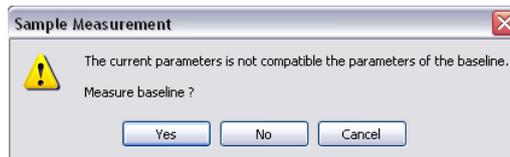


Figure. 6.6 Message box for sample measurement

Click <Yes>, and the baseline measurement is carried out using the current parameters. Click <No>, and the baseline measurement is carried out using different measurement condition. Click <Cancel>, and the baseline measurement is interrupted and waits for next instruction. When the measurement has to do emergency stop, click  or select [Cancel] in the [Measure] menu.

CASE B: If baseline measurement is not completed, the sample is measured without baseline correction.

**Note (1):** *Suspending measurement displays a spectrum from [Start] to measured wavelength in the View. This is also the same with the case that the [Cycle Times] is selected.*

**Note (2):** [Baseline] or [Blank] measurement should be completed for the purpose obtaining baseline corrected sample data.

**Note (3):** The same measurement parameters between sample and baseline measurement should be employed.

### 6.3.5 Saving Data

**Note :** Refer also to Section 5.1.1.

#### 6.3.5.1 Saving Parameters

Saves parameters given to disk.

**Note :** Save parameters when the parameter setting is activated.

- (1) Click [Save Parameters...] from the [File] menu, which is on the [Time Course Measurement] screen. Click  is can be used. The following dialog box appears.

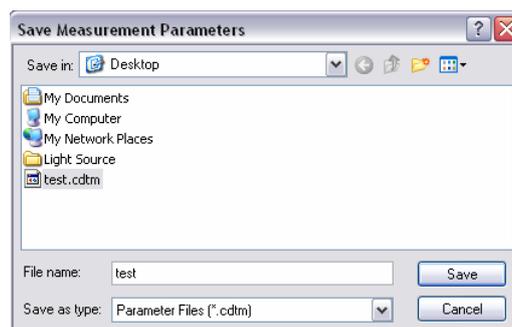


Figure. 6.7 [Saving Parameters] dialog box

- (2) Select a location to save the spectrum clicking the arrow at extreme right in the [Save in] box. (In Fig. 6.7, “Desktop” is selected)
- (3) Input a filename into the [File Name] text box. The extension (after ".") need not be entered. The output file is saved as a .cdtm format file.
- (4) Click the <Save> button, and the spectrum is saved to disk. (File name of Fig. 6.7 is “test”)

### 6.3.5.2 Saving Sample Data

Saves a measured sample data to disk.

**Note :** *Save it when the sample measurement is completed.*

- (1) Click [Save Data...] from the [File] menu, which is on the [Time Course Measurement] screen. Clicking  is also the same. The following dialog box appears.

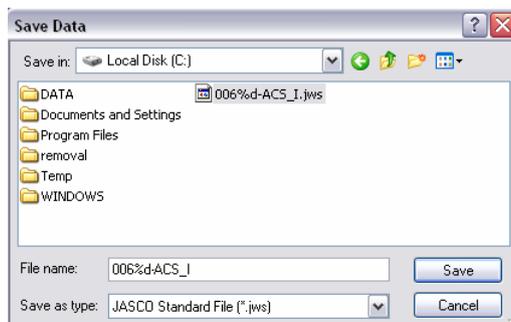


Figure. 6.8 [Saving Data] dialog box

**Note :** *The [Save data] is available after sample measurement is completed or sample data is loaded onto the [Time Course Measurement].*

- (2) Select a location to save the data clicking the arrow at extreme right in the [Save in] box. (In Fig. 6.8, “Local Disk (C)” is selected)
- (3) Input a filename into the [File Name] text box. The extension (after ".") need not be entered. The output file is saved such as xxx.jws.
- (4) Clicking the <OK> button saves the spectrum to disk. (filename of Fig. 6.7 is “0.06%d-ACS\_I)
- (5) In the case that the [Cycle Times] was selected, “Cycle Times”= 3, for example, three data are memorized as xxx\_01.jws, xxx\_02.jws, and xxx\_03.jws.

**Note :** *Suspending measurement data is saved form [Start] to where interrupted. This is also the same with the case that the [Cycle Times] is selected.*

### 6.3.6 Sending Spectrum to [Spectra Analysis]

Sends a measured spectrum into the [Spectra Analysis] window.

- (1) Click [Analysis Send] from the [File] menu or  in the [Spectra Measurement] window. The [Spectra Analysis] window is automatically opened.
- (2) When [Cycle Times] is selected, the following dialog box appears after clicking [Analysis Send]. (In Fig. 6.9, Cycle Times is set to be 3)

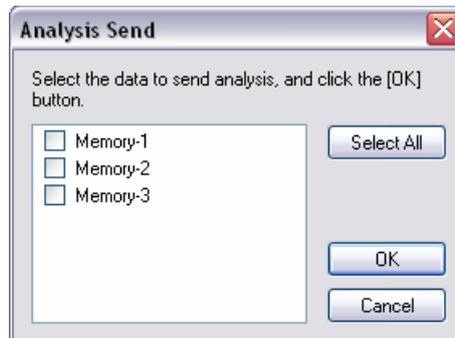


Figure. 6.9 [Save As...] dialog box

- (3) Check marks in the boxes of Fig. 6.10 and click <OK> button. The selected data are sent to [Spectra Analysis]. All data can be sent to [Spectra Analysis] by clicking <Select All>.

**Note :** *If sample data is not memorized (see [Save Data]), the filename is given automatically such as “Memory”. In the case [Cycle time] is given, the filenames are given as “Memory-1”, “Memory-2”, “Memory-3”... (See Fig.4.10) When sample data is memorized, the registered name is employed in spite of “Memory”.*

### 6.3.7 Printing Spectrum

The measured spectrum is printed out. This is available in the [Spectra Analysis] window. Click [Print...] from the [File] menu, and printing out is carried out. [Print Setup...] is useful when the output title is needed.

**Note :** *Refer to “Spectra Analysis manual” for more detail.*

## 7 Operation of Spectra Analysis Program

In this section, the usage of special analysis functions for the J-810/815 from a common platform is described. Refer to the [Spectra Analysis] manual for more information.

### 7.1 Starting the spectra analysis program

*Note: If spectra analysis is performed after spectrum measurement, startup operation is unnecessary. Refer to Sections 3 and 5 for how to start the spectra analysis program from the measurement program.*

Double click the [Spectra Analysis] icon in the [Spectra Manager] program. The spectra analysis program displays the following window when it starts.

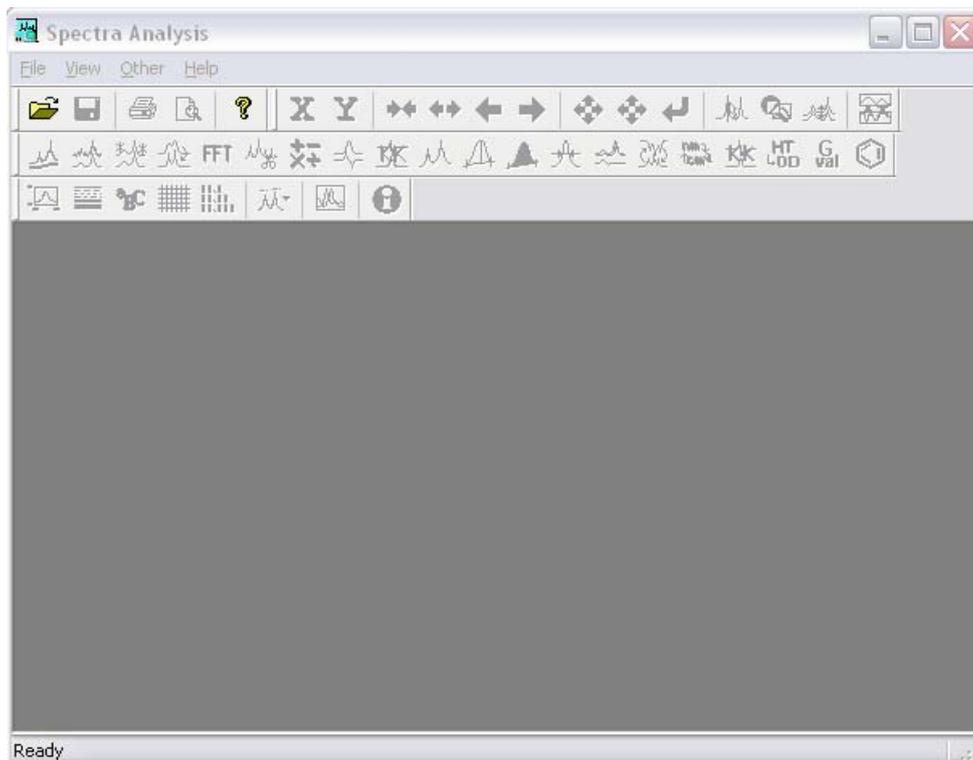


Figure 7.1 [Spectra Analysis] window

## 7.2 Loading spectra

A spectrum saved on disk can be loaded to the View display of the spectra analysis program and it can be saved on disk. There are two types of files: JASCO Standard files (.jws) and JASCO Old Standard files (.jws and .txt).

### 7.2.1 Opening JASCO Standard file

- (1) Select [Open] from the [File] menu. The following dialog box appears.

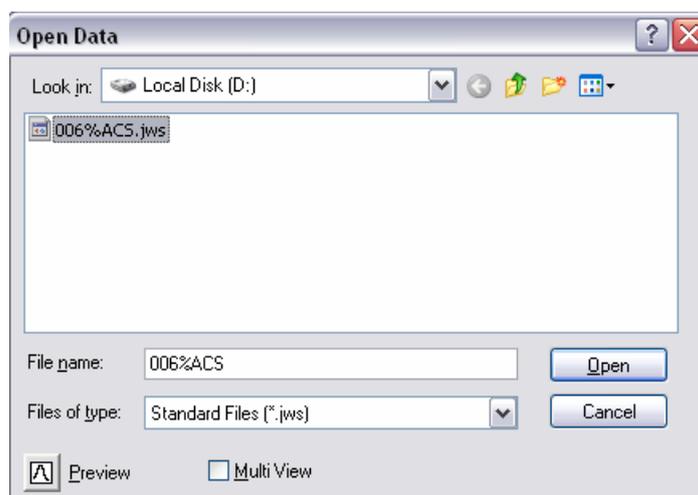


Figure 7.2 [Open New File] dialog box

- (2) Click on the file name from the [File Name] list (“006%ACS.jws”, for example).
- (3) Click on the <Open> button. A new View opens and the selected spectrum is displayed.

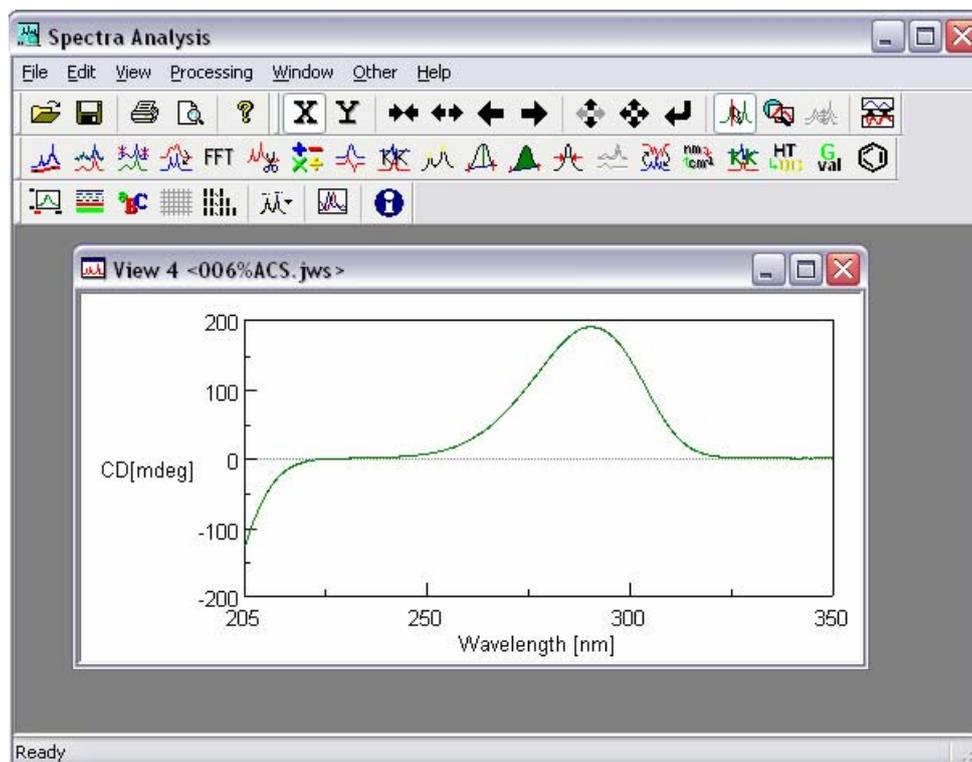


Figure 7.3 Spectrum View

## 7.2.2 Opening JASCO Old Std file

- (1) Click on [Import] in the [File] menu. The following dialog box appears.

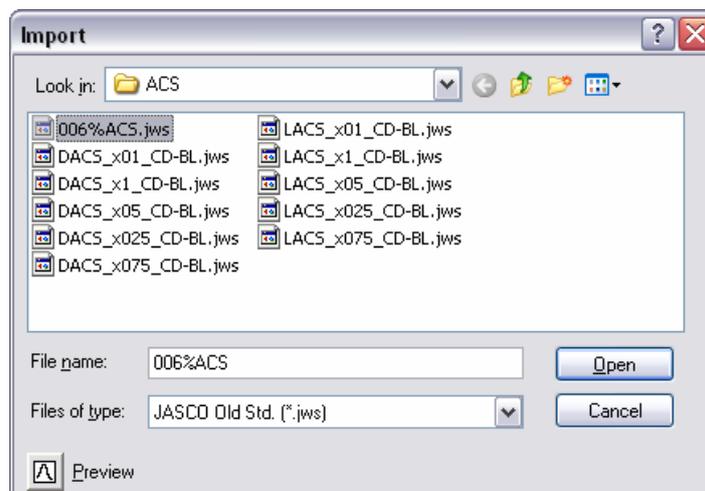


Figure. 7.4 [Open New File] dialog box

- (2) Click on a file name from the [File Name] list (“006%ACS.jws”, for example).
- (3) Click on the <Open> button. A new View such as the one shown in Fig. 7.3 opens.

**Note (1):** ASCII files (.txt) and JCAMP-DX files (.dx) are opened from [Import] in the [File] menu, which are the [Files of type] menu shown in Fig. 7.4.

**Note (2):** Imported files can be transferred by saving them as JASCO Standard files.

## 7.2.3 Saving as JASCO Standard file

- (1) Click on [Save] or [Save As] in the [File] menu. The following dialog box appears.

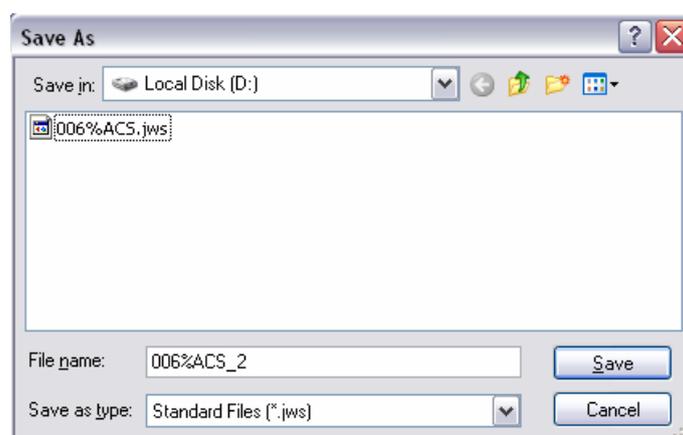


Figure 7.5 [Open New File] dialog box

- (2) Enter the file name into the [File Name] box (“006%ACS\_2.jws”, for example).
- (3) Click on the <Save > button. The JASCO standard file is saved on the Local Disk (D:).

## 7.2.4 Saving as JASCO Old Std file

- (1) Click on [Export] in the [File] menu. The dialog box of Figure 7.5 appears.
- (2) Enter the file name into the [File Name] box and click on the <Save> button. The JASCO Old std file is saved on the Local Disk (D:).

**Note (1):** The spectra in the View window can be saved as an ASCII file (.txt) and as a JCAMP-DX file. Select the file type from the [Save as type] menu of Fig. 7.5.

## 7.3 Calculation menus unique for the J-810/815

[CD Options] and [Common Options] are included in the Spectra Analysis program for J-810/815.

### 7.3.1 CD options

The following menus are included in [CD Options] in the [Processing] menu.

[CD Options] menu

- [KK Conversion...]: Converts CD spectra into ORD spectra or ORD spectra into CD spectra.
- [HT -> OD...]: Calculates Abs spectra using HT spectra.
- [G-Value...]: Calculates G-value using both CD and Abs spectra.
- [Optical Constant...]: Transforms CD (mdeg) into molar ellipticity, delta OD, molar CD, and specific ellipticity.

#### 7.3.1.1 K-K conversion

- (1) Load a JASCO standard or JASCO Old Std file into the Spectra Analysis Window using the procedure described in Section 7.2 (see Fig. 7.3).
- (2) Select [Processing] - [CD-Options] - [KK Conversion...]. The following dialog box appears.

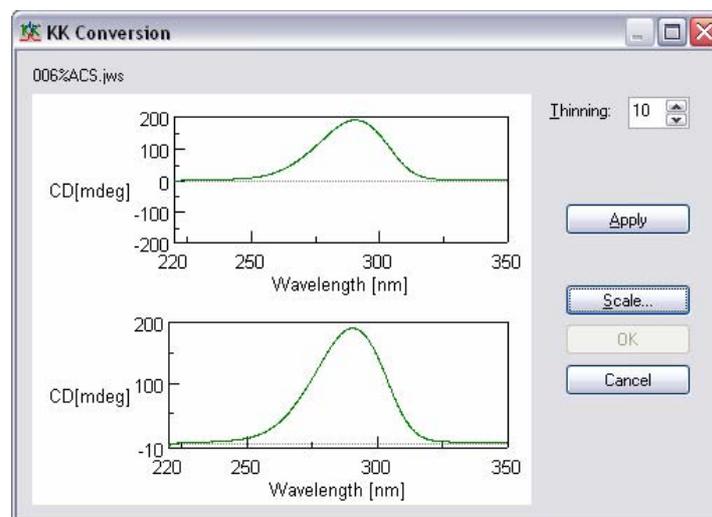


Figure 7.6 [KK Conversion] dialog box

- (3) Click on the <Apply> button, and the dialog Fig. 7.6 is changed as Fig. 7.7.

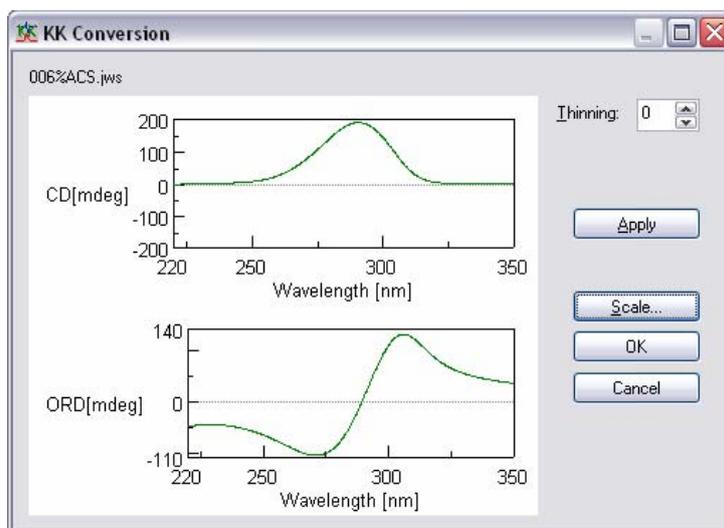


Figure 7.7 [KK Conversion] dialog box

#### Other functions

[Scale]: This is used for defining the wavelength region for K-K conversion. Click on the <Scale> button and the following dialog box appears.

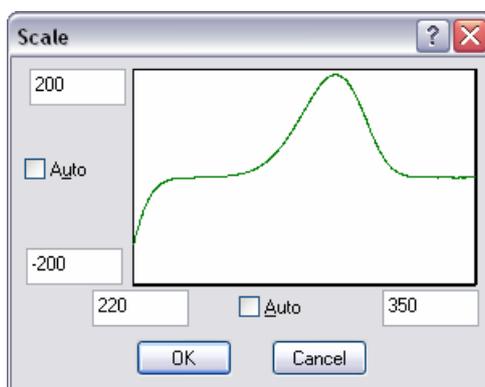


Figure 7.8 [KK Conversion] dialog box

[Thinning]: Adjusts the data pitch by [Thinning:] values. The data pitch of an ORD spectrum is defined as  $\text{CD data pitch} \times \text{thinning value}$ . When the [Thinning:] value is set to 0, the same data pitch is defined with the reference data. [Thinning] can be changed by clicking the arrow on the extreme right of the [Thinning] box.

[Apply]: performs the K-K conversion.

[OK]: Sends the calculation result into the View.

[Cancel]: Stops the operation and returns to the view of loaded file (Fig. 7.3).

### 7.3.1.2 HT -> OD

- (1) Load a JASCO standard or JASCO Old Std file into the Spectra Analysis Window following the procedure described in Section 7.2 (see Fig. 7.3).

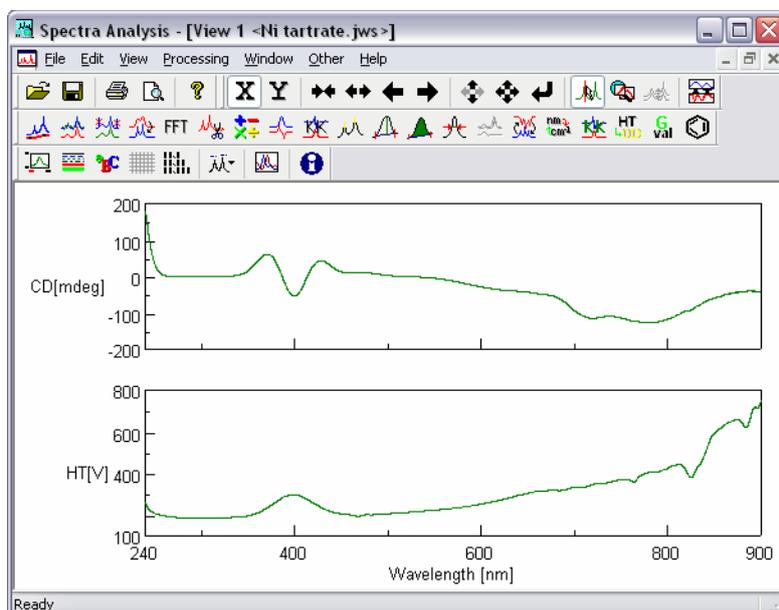


Figure 7.9 Spectrum View (before calculation)

- (2) Click on [Processing] - [CD-Options] - [HT->OD...]. The HT spectrum displayed in channel #2 is converted into an Abs spectrum (see Fig. 7.10).

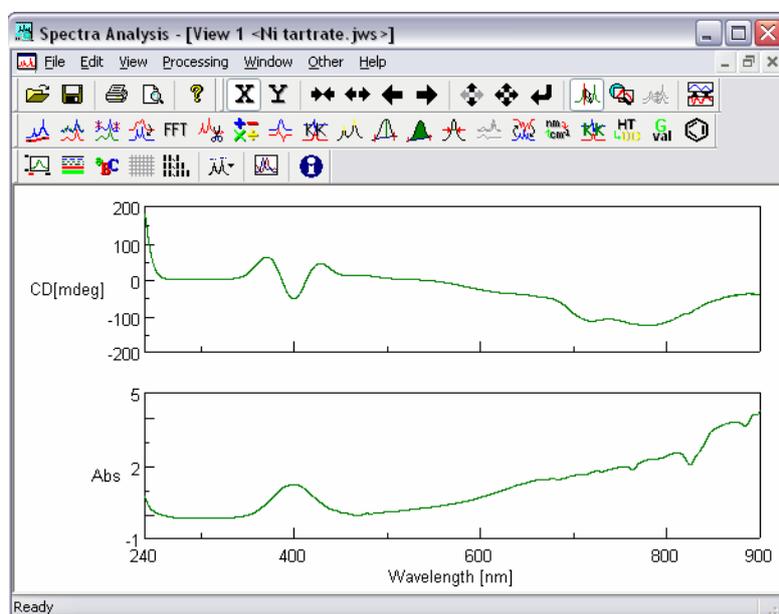


Figure 7.10 Spectrum View (after calculation)

- (3) Steps (1) and (2) should be repeated for the baseline spectrum.
- (4) Subtract the baseline Abs spectrum from the sample Abs Spectrum using [Arithmetics with Data] in [Common Option] of [Processing].

### 7.3.1.3 G-value

- (1) Load a JASCO standard or JASCO Old Std file into the Spectra Analysis Window following the procedure described in Section 7.2. In this case, the loaded spectra is an Abs spectrum (see Fig. 7.11).

**Note (1):** G-value calculation needs an Abs spectrum. So, the loaded spectrum must include an Abs spectrum. Do not forget this.

**Note (2):** The Abs spectrum must be baseline corrected. If not, the G-value will be incorrect.

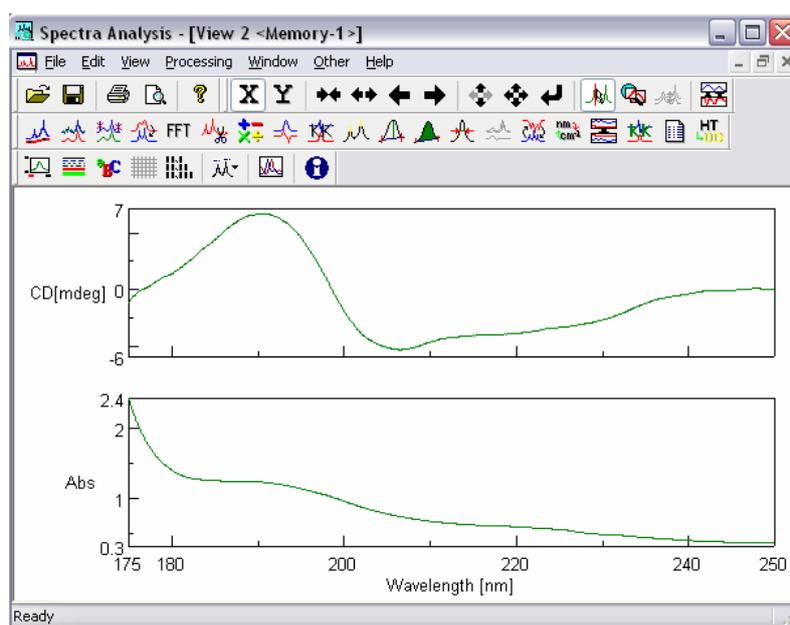


Figure 7.11 Spectrum View for G-value calculation

- (2) Click on [Processing] - [CD-Options] - [G-value...]. G-value, CD, and Abs are displayed as shown in Fig. 7.12 (see below).

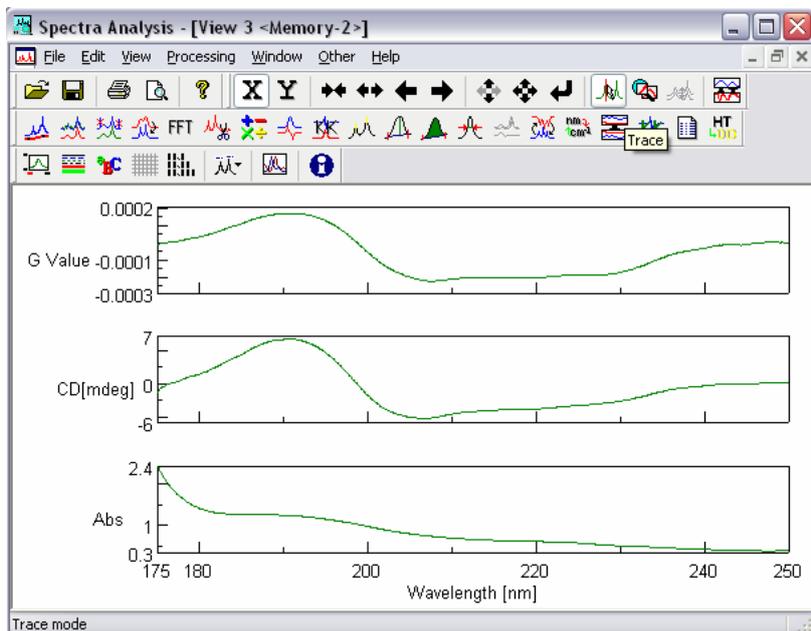


Figure 7.12 Spectrum View for G-value calculation

**Note:** Figure 7.12 is shows test data. The actual G-value is different.

### 7.3.1.4 Optical Constant

- (1) Load JASCO standard or JASCO Old Std file into the Spectra Analysis Window using the procedure described in Section 7.2. The spectrum is displayed in the View.
- (2) Click on [Processing] – [CD options] – [Optical Constant]. The following dialog box appears.

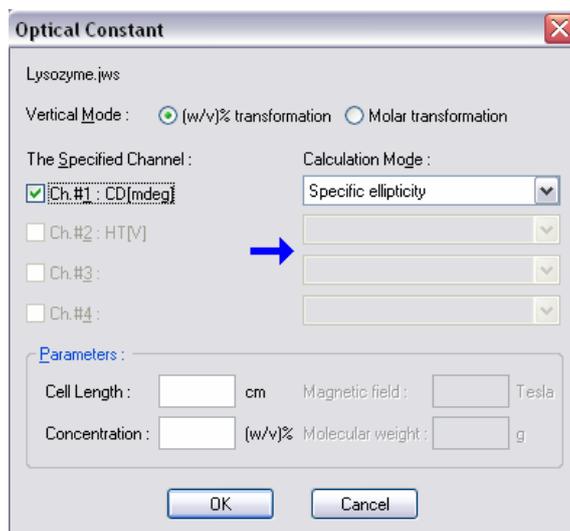


Figure 7.13 [Optical Constant] dialog box

- (3) Select [(W/V)% transformation] or [Molar transformation] as desired.
- (4) Put a check mark in the Ch # box where CD (mdeg) is displayed (CH#1 in Fig. 7.13, for example).
- (5) Enter the desired cell length (cm) and the concentration (w/v)% in the [Cell Length] and the [Concentration] boxes.
- (6) Click the <OK> button. The [CD] is changed into [Spc. Ellip.] (see Fig. 7.14).

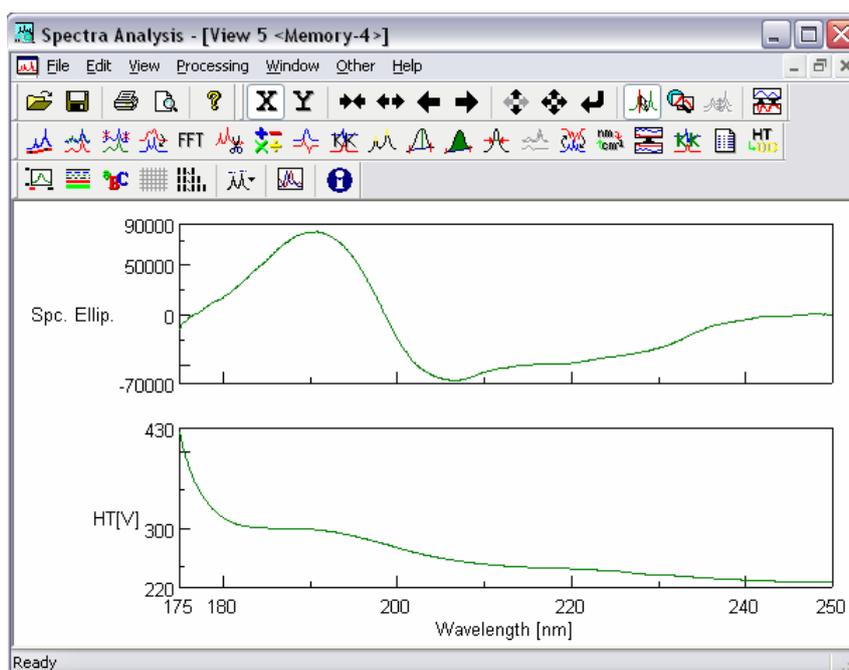


Figure 7.14 Spectrum View (after calculation)

**Note(1):** The parameters needed for the calculation are shown with active boxes (gray parameters are not necessary). In the case of the [Spc. Ellip.] calculation, [Cell Length] and [Concentration] are needed, but [Magnetic field] and [Molecular weight] are not necessary.

**Note(2):** The following calculations are supported: Specific ellipticity, magneto specific ellipticity,  $\Delta OD$ , molar ellipticity, magneto molar ellipticity,  $\Delta OD$ , molecular CD, and magneto molecular CD. These are performed by following the same procedure described in steps (1)-(6).

## 7.3.2 Common Options

The following menus are collected under [Common Options] in the [Processing] menu.

[Common Options] menu

- [Channel Conversion...]: This is used for changing the channels that spectra are displayed on (Ch #1 = CD and Ch #2 = HT becomes into Ch #1 = HT and Ch #2 = CD, for example). It is also possible to extract each spectrum.
- [Data Dump...]: Shows and copies digital data, CD, HT, Abs, etc.
- [Data Accumulation...]: Produces an averaged spectrum. It requires several spectra all having the same axis units.
- [Arithmetic with Channel...]: Performs the four arithmetic operations on the same channel between different data.
- [Arithmetic with Data...]: Performs the four arithmetic operations between channels for one data set.

### 7.3.2.1 Channel Conversion

- (1) Load a JASCO standard or JASCO Old Std file into the Spectra Analysis Window using the method described in Section 7.2. Fig. 7.15 is an example.

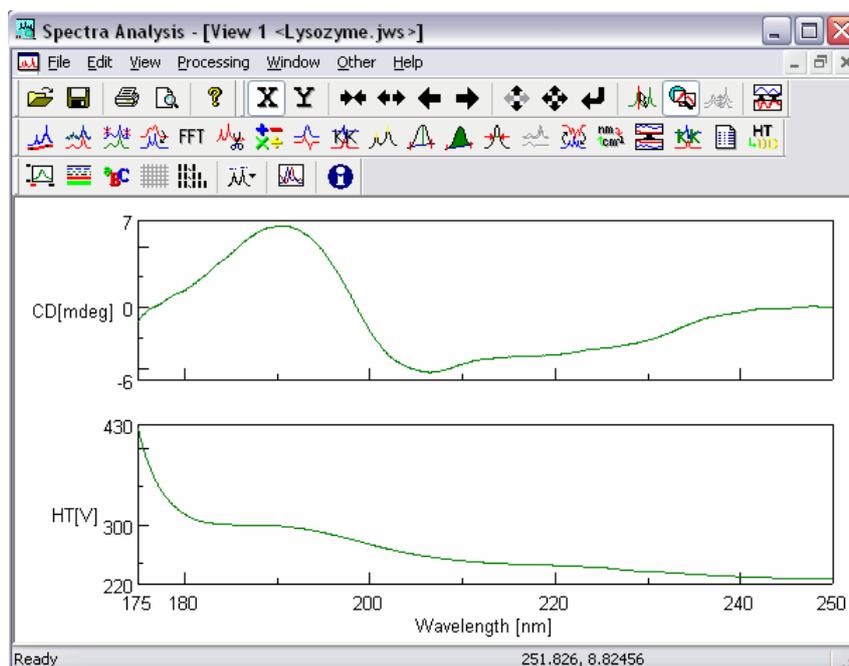


Figure 7.15 Spectrum View (before operation)

- (2) Click on [Processing] - [Common-Options] - [Channel Conversion...]. The following dialog box appears.

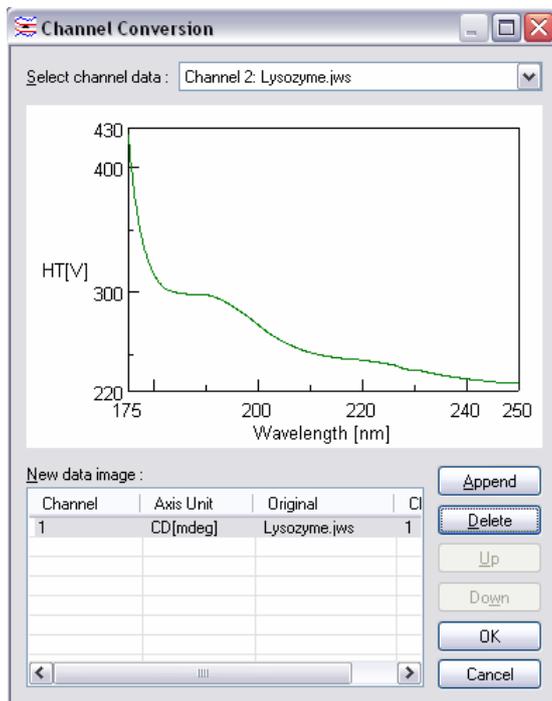


Figure 7.16 [Channel Conversion] dialog box

- (3) Select the desired spectrum from the list in [Selected channel data] (located at the top of the dialog box shown in Fig. 7.16). Clicking the arrow on the extreme right displays the list.
- (4) Click the <Append> button. The selected spectrum is listed in [New data image] view (see Fig. 7.16, for example).

- (5) Click the <OK> button. The following spectrum is obtained.

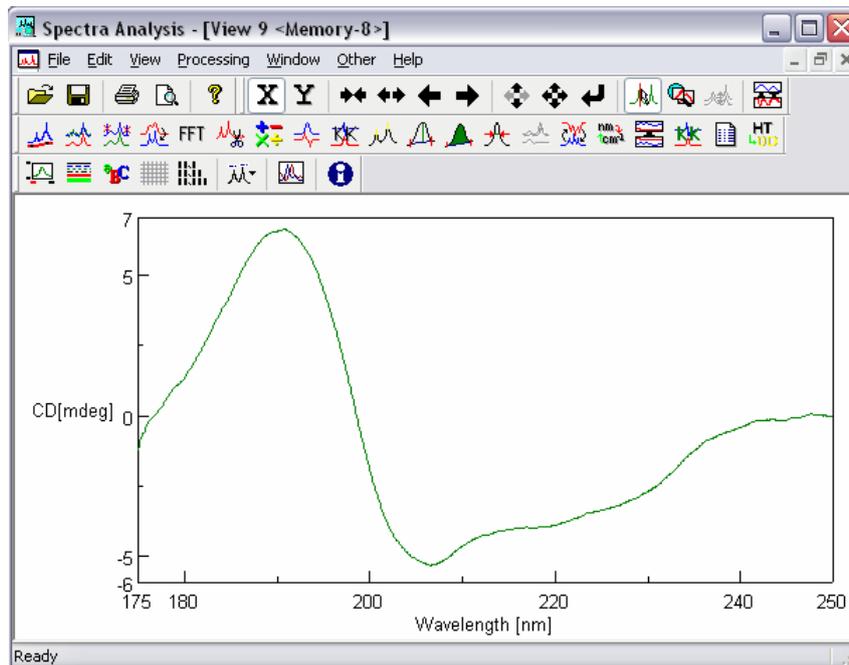


Figure 7.17 Spectrum View (after operation)

Spectra can be rearranged.

- (6) Update the selected file by repeating the procedure from step (3) (click the <Append> button in the dialog box shown in Fig. 7.16). Fig. 7.16 becomes as follows.

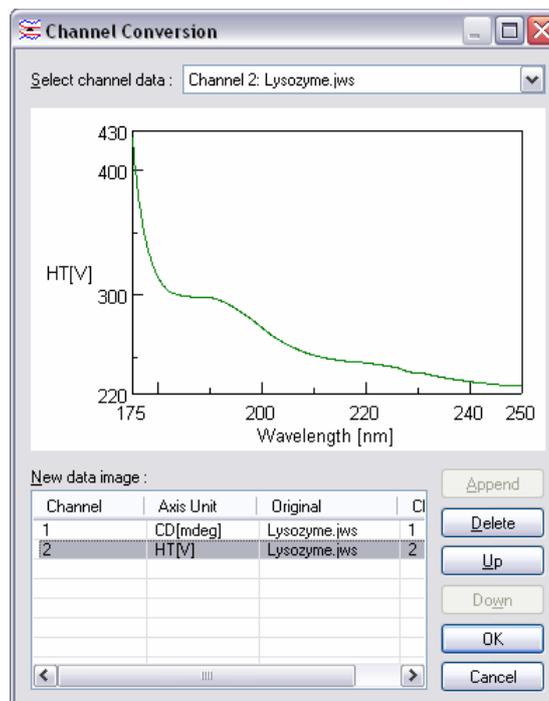


Figure 7.18 [Channel Conversion] dialog box

- (7) Click on the <Up> or <Down> buttons results in the channel number of the target spectrum (HT in Fig. 7.18) increasing (#2 -> #1) or decreasing (#1 -> #2), respectively.
- (8) Click on the <OK> button of Fig. 7.18. The following data is obtained.

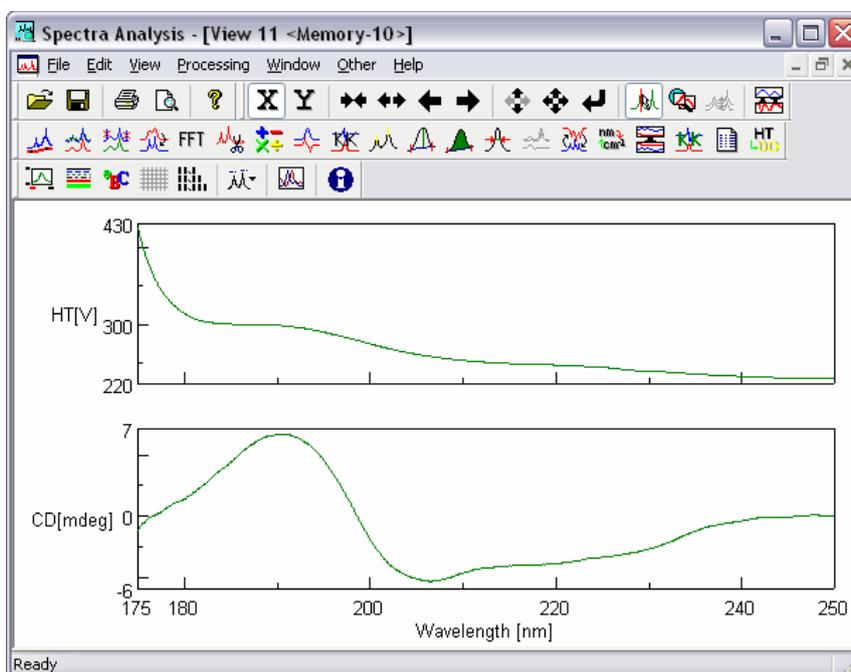


Figure 7.19 Spectrum View (after operation)

The content of ch# can be selected from several different files. This is performed by overwriting several loaded files following the procedure (1) and following steps (2) – (7). Figure 7.20 shows an example, where ch#1 and ch#2 is CD (mdeg) and Mol. Ellip., which are extracted from different files.

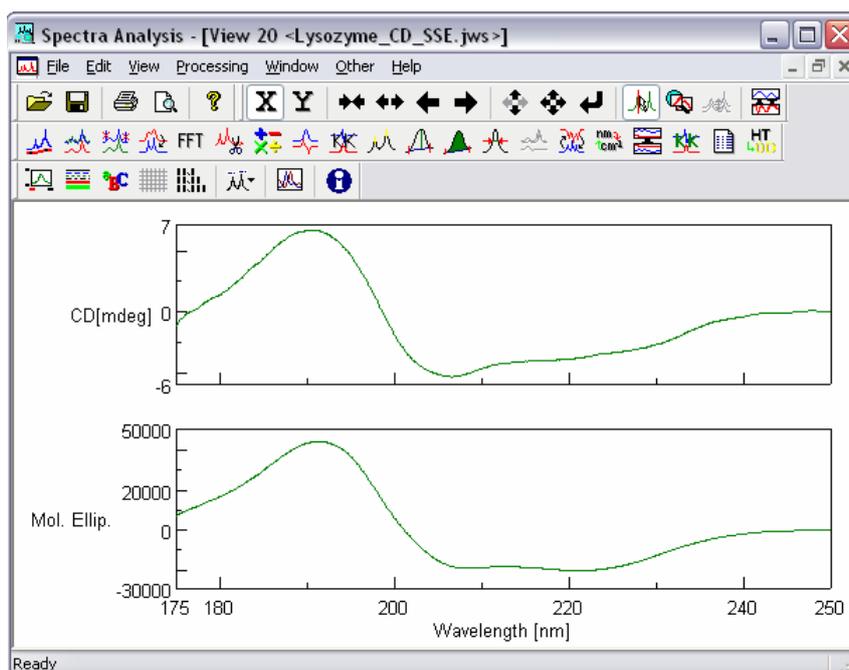


Figure 7.20 Spectrum View (after the operation)

### 7.3.2.2 Data Dump

- (1) Load a JASCO standard or JASCO Old Std file into the Spectra Analysis Window following the procedure described in Section 7.2. Figure 7.21 shows an example.

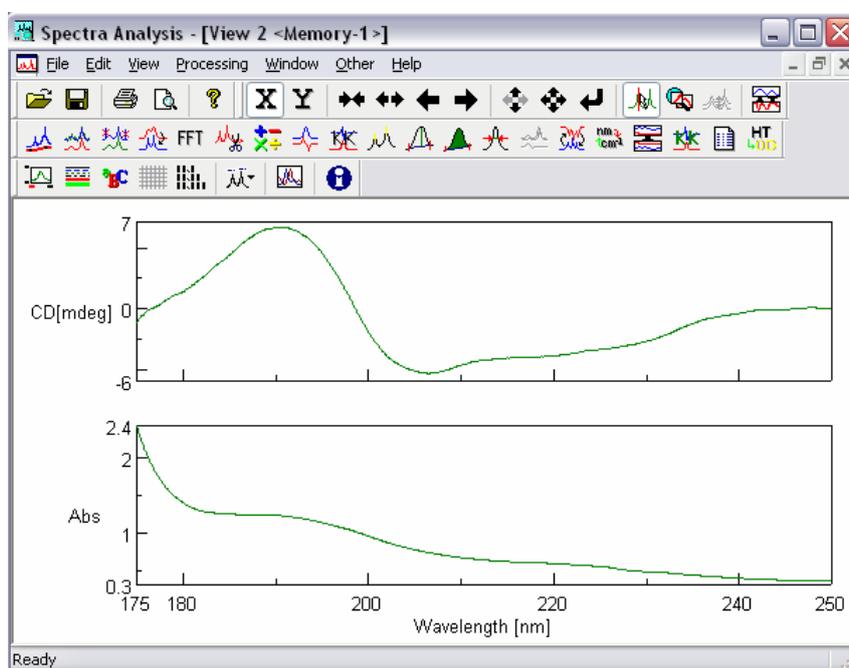


Figure 7.21 Spectrum View

- (2) Click on [Processing] - [Common-Options] - [Data Dump...]. The following dialog box appears.

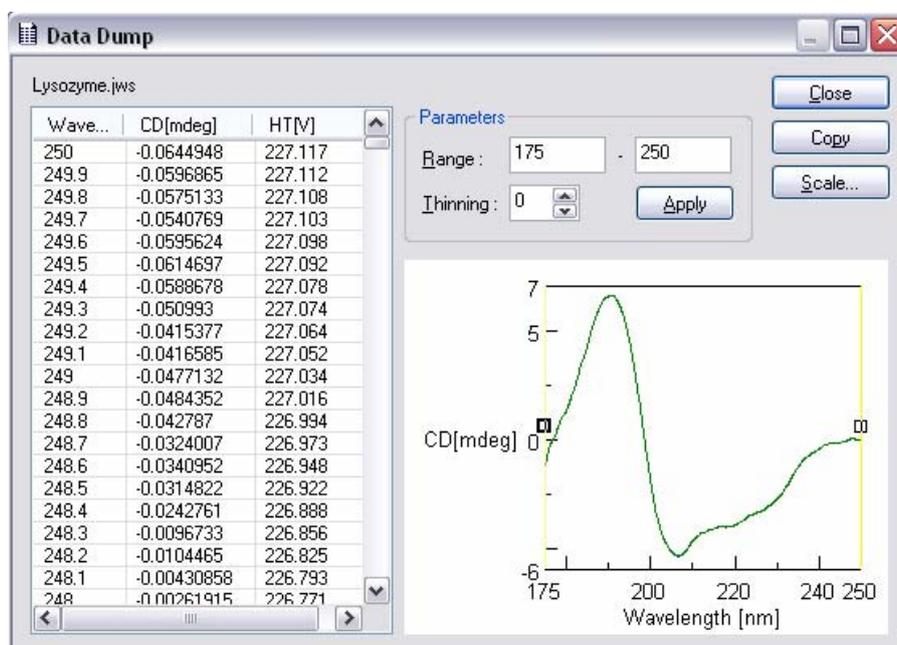


Figure 7.22 [Data Dump] dialog box

- (3) Click on the <Apply> button. The digital data, wavelength, CD and HT are displayed on the left side of the dialog box (see Fig. 7.22).

#### Other functions

[Scale]: Refer to Section 7.3.1.1 (see Fig. 7.8).

[Thinning]: Refer to Section 7.3.1.1.

[Copy]: Reads the digital data wavelength, CD and HT which are displayed on the left side of the dialog box (see Fig. 7.22). These can be pasted into a text file (Notepad, Wordpad, Word, etc...).

[Range]: Sets the wavelength range for displaying the data.

[Apply]: Applies the wavelength range set by the [Range].

### 7.3.2.3 Data Accumulation

- (1) Load several JASCO standard or JASCO Old Std files into the Spectra Analysis Window following the procedure described in Section 7.2.
- (2) Overwrite these data (refer to the “Spectra Analysis” Manual).
- (3) Click on [Processing] - [Common-Options] - [Data Accumulation...]. Accumulation is performed and the accumulated data is displayed in the View.

**Note:** Vertical and horizontal axis units and the wavelength range must be the same.

### 7.3.2.4 Arithmetic with Channel

- (1) Load several JASCO standard or JASCO Old Std files into the Spectra Analysis Window following the procedure described in Section 7.2. We used the data of Fig. 7.20 here, as an example (file name is “Lysozyme\_CD\_SSE.jws”).
- (2) Click on [Processing] - [Common-Options] - [Arithmetic with Channel...]. The following dialog box appears.

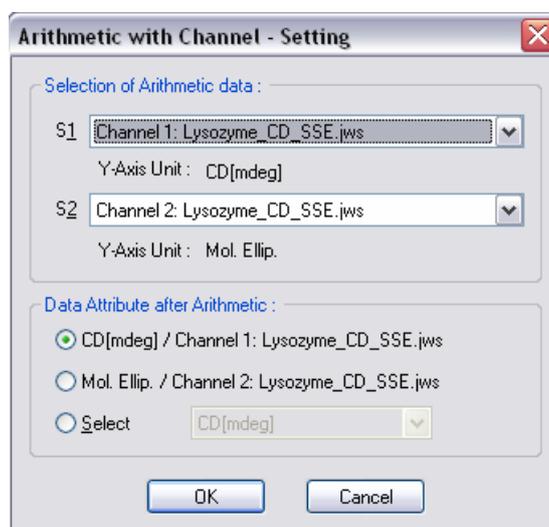


Figure 7.23 [Arithmetic with Channel - Setting] dialog box

- (2) Select the ch# for S1 and S2. Clicking the arrow on the extreme right displays a list of S1 and S2.
- (3) Set the vertical axis unit after the calculation. Select either [/Channel 1], [/Channel 2], or [Select]. When [Select] is selected, a selection of units are available, which are displayed by clicking the arrow to the extreme right of the [Select] box.
- (4) Click on the <OK> button of Fig. 7.23. The following view is displayed (the vertical axis unit was set to be A.U.).

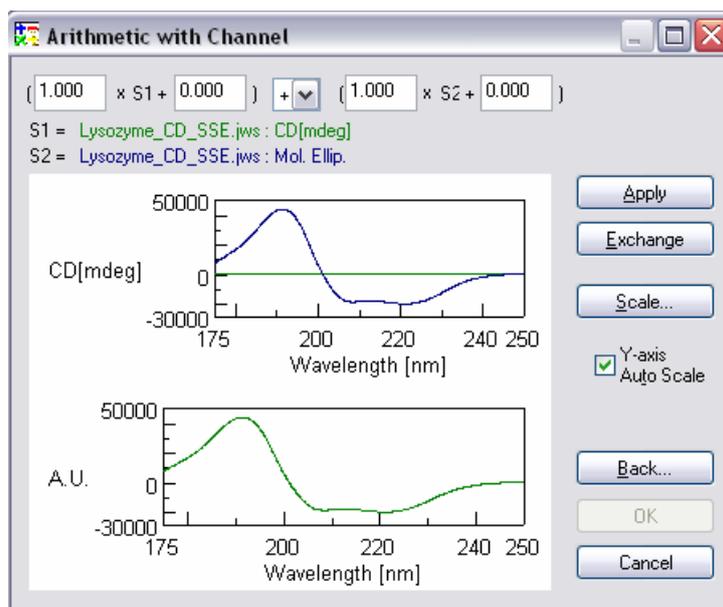


Figure 7.24 [Arithmetic with Channel] dialog box

- (5) Enter appropriate values into the boxes on the top of the dialog box. Select the operation by clicking the arrow at the top of the dialog box.

- (6) Click on the <Apply> button. The A.U. spectrum of Fig. 7.24 appears as follows (the operation “/” was selected in this example).

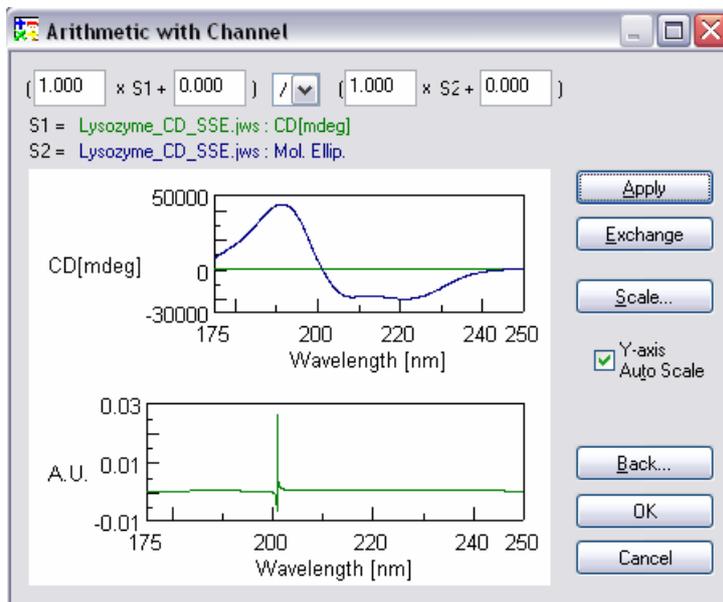


Figure 7.25 [Arithmetic with Channel] dialog box

- (7) Click on the <OK > button, and the A.U. spectrum is displayed in the View window.

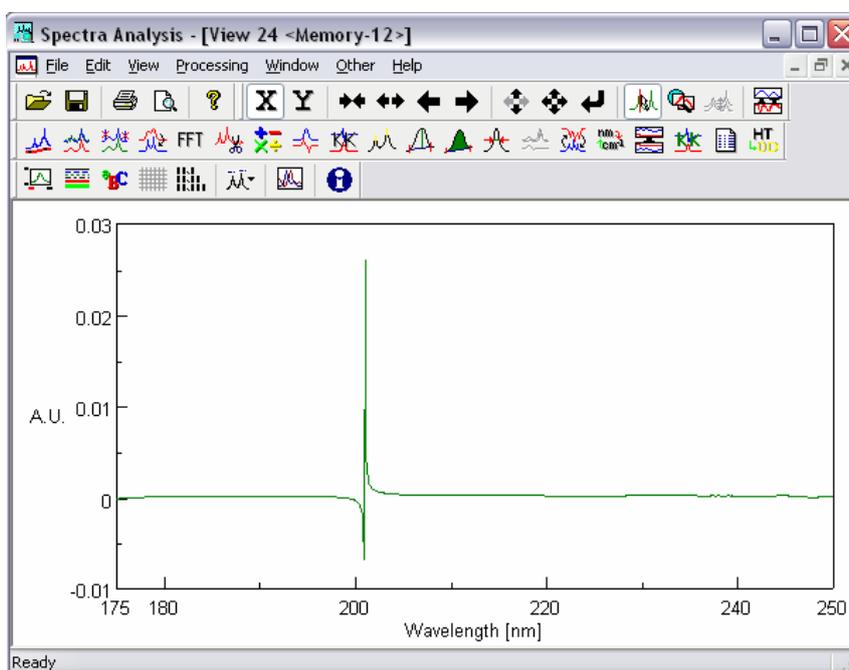


Figure 7.26 Spectrum View (after calculation)

Other functions

[Scale]: Refer to Section 7.3.1.1 (see Fig. 7.8).

- [Exchange]: Exchanges the contents of S1 and S2. Click on the <Exchange> button of Fig. 7.25, for example, the contents S1 and S2 becomes Lysozyme\_CD\_SSE.jws : Mol. Ellip. and Lysozyme\_CD\_SSE.jws : CD[mdeg], respectively.
- [Back]: Returns to the dialog box shown in Fig. 7.24 or 7.25.
- [Cancel]: Stops the operation and returns to the view of loaded file (see Fig. 7.24 or 7.25).
- [Y-axis Auto Scale]: Automatically adjusts the vertical axis. Insert a check mark in the box.

### 7.3.2.5 Arithmetic with Data

- (1) Load several JASCO standard or JASCO Old Std files into the Spectra Analysis Window following the procedure described in Section 7.2. Figure 7.20 data is used here, for example (File name is "Lysozyme\_CD\_SSE.jws").
- (2) Click on [Processing] - [Common-Options] - [Arithmetic with Data...]. The following dialog box appears.

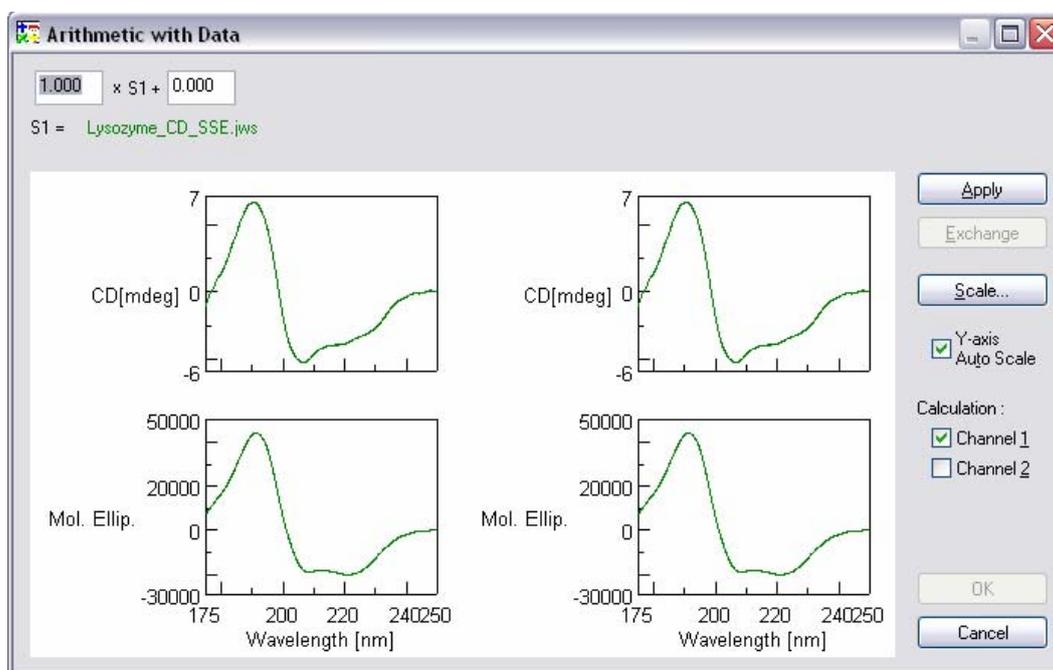


Figure 7.27 [Arithmetic with Data] dialog box (before calculation)

- (3) Insert appropriate values in the boxes displayed at the top of the dialog. Insert a check mark in the [Channel 1] and/or [Channel 2] as desired.

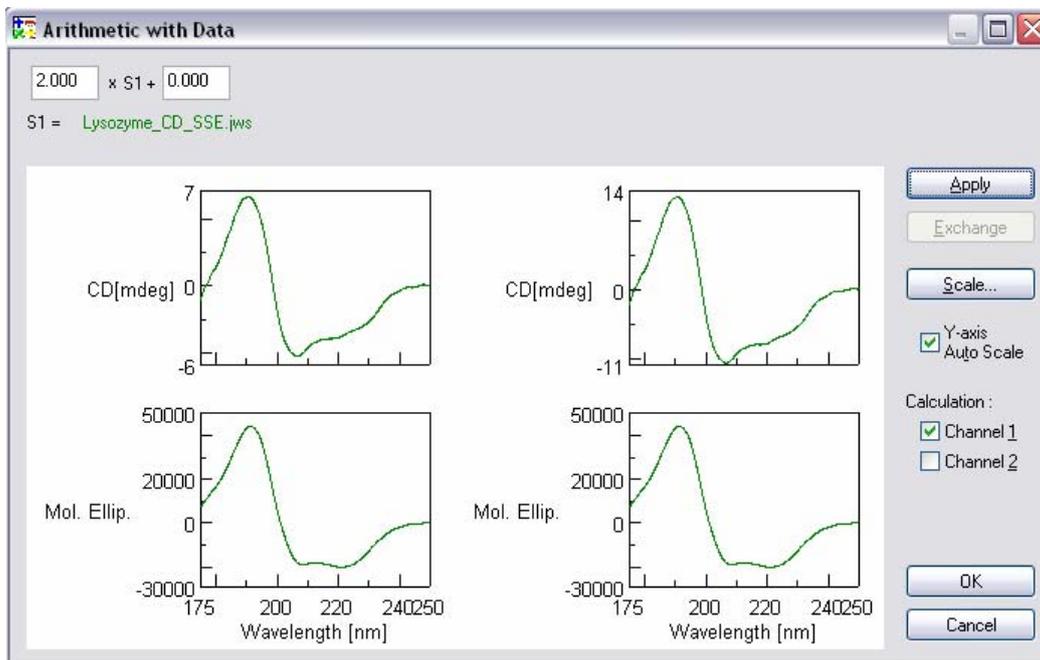


Figure 7.28 [Arithmetic with Data] dialog box (after calculation)

- (4) Click on the <OK > button, and the calculated spectrum is displayed in the view window.

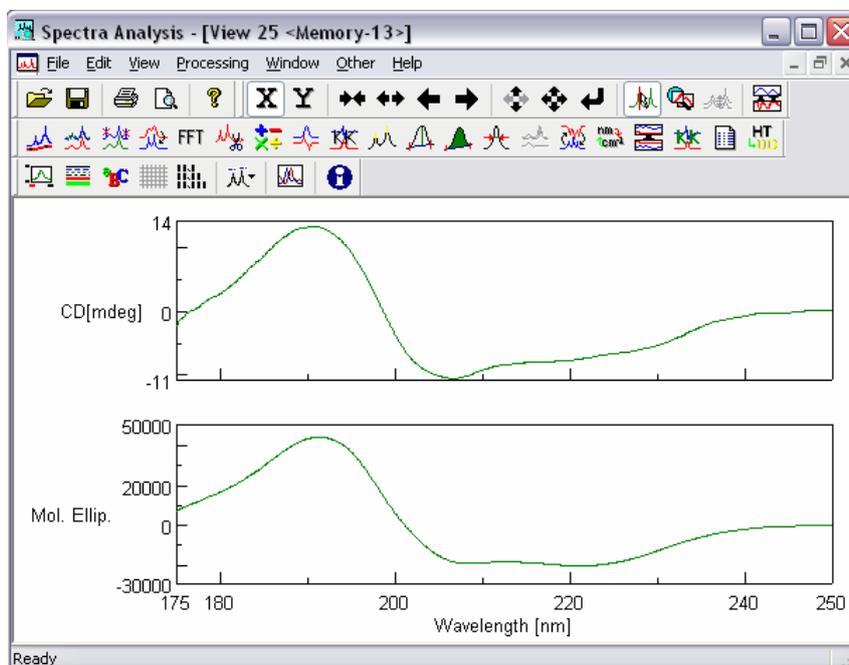


Figure 7.29 Spectrum View

Other functions

- [Scale]: Refer to Section 7.3.1.1 (see Fig. 7.8).
- [Exchange]: Exchanges the contents of S1 and S2. Click on the <Exchange> button shown in Fig. 7.27 or 7.28 for example, the contents of S1 and S2 become Lysozyme\_CD\_SSE.jws : Mol. Ellip. and Lysozyme\_CD\_SSE.jws : CD[mdeg], respectively.
- [Cancel]: Stops the operation and returns to the view of loaded file.

## 7.4 Closing Spectra Analysis Programs

### (1) Closing spectra analysis program

Upon completion of a series of analyses, click on [File] - [Exit]. The [Spectra Analysis] window disappears and the [Spectrum Measurement] window appears from below.

**Note:** *If there are any unsaved spectra open in the window, a message will appear to that effect. Take appropriate action to the message. The message will appear for as many number of times as there are number of unsaved spectra. Repeat this procedure appropriately.*

### (2) Closing the [Spectra Manager] program

Click on [Application] - [Exit].

## 8. Appendix

Parameters selected can seriously affect measurement results. The following summarizes how to select parameters.

- (1) **Measuring wavelength range**  
Most CD spectrum peaks appear in a specific wavelength region (short wavelength region as with ultraviolet-visible absorption spectra with most organic compounds). If the optically active absorption band position of sample is known, make measurement from 50 to 100 nm before the leading end of the spectrum to the trailing end of the spectrum where it converges at zero, though it slightly varies with the width and shape of the spectrum.
- (2) **Data acquisition intervals (resolution)**  
<In Spectra Measurement>  
Usually, about 0.2 nm will do. However, if the scanning speed is set at [Step], about 1 nm is appropriate. Make the resolution coarse if spectrum peaks are broad or fine if sharp.  
<In time course measurement>  
Make the resolution fine in a measurement where the time course change is quick.
- (3) **Scanning speed**  
The scanning speed must be changed according to D.I.T.. Usually, set the scanning speed at 20 to 100 nm/min and D.I.T. at 0.25 to 2 sec in measurement. Table 8.1 shows a guide of D.I.T. with respect to scanning speed.

Table 8.1 Guideline of D.I.T. vs. Scanning Speed

Scanning speed (nm/min)	D.I.T. (recommended)	Higher limit
10000	1.0 to 2.0 msec	32.0 msec
5000	2.0 to 4.0 msec	64.0 msec
2000	4.0 to 8.0 msec	0.25 sec
1000	32.0 msec to 0.125 sec	0.5 sec
500	64.0 msec to 0.25 sec	1.0 sec
200	0.125 to 0.5 sec	2.0 sec
100	0.25 to 1.0 sec	4.0 sec
50	0.5 to 2.0 sec	8.0 sec
20	1.0 to 2.0 sec	16.0 sec
10	2.0 to 4.0 sec	16.0 sec
5	2.0 to 8.0 sec	16.0 sec
2	4.0 to 16.0 sec	16.0 sec
1	8.0 to 16.0 sec	16.0 sec

- (4) **No. of integration**  
The following relationship holds between signal-to-noise ratio and No. of integration. Increasing the No. of integration improves signal-to-noise ratio of spectrum. Determine it by taking into account the spectrum (sample) condition and measurement time (increasing the No. of integration prolongs measurement time).  
If sensitivity is lower than 100 mdeg/FS, one integration will do.  
Table 8.2 shows guidelines of No. of integration when a sample with absorbance 1 or less is measured with a D.I.T. of 2 sec.

Table 8.2 No. of Integration and Sensitivity (D.I.T. 2 sec)

Sensitivity (CD mdeg/FS)	No. of integration
50	1 - 2
20	4
10	4 - 8
5	4 - 16
2	8 - 32
1	16 - 50

**Note:** In time course measurement, set the time to 1. Integration can be used in stopped flow measurement (see the instruction manual for the stopped flow unit).

(5) D.I.T.

<In Spectra Measurement>

The following relationship holds between D.I.T. and signal-to-noise ratio. The signal-to-noise ratio of a spectrum measured for four seconds is twice that for one second. Data at a given point is the average value of sampling data before and after that time (D.I.T./2). Therefore, the longer the D.I.T., the greater the effect of previous data on the current data. Do not increase D.I.T. excessively if scanning is made at a high speed or if resolution is lowered.

Table 8.3 shows D.I.T. to obtain a spectrum of high signal-to-noise ratio at a desired sensitivity. If sensitivity is higher than 20 mdeg/FS, setting D.I.T. at 1 to 2 seconds and increasing the number of integration to improve signal-to noise ratio is very effective because spectra are averaged simultaneously.

Table 8.3 D.I.T. to Obtain High Signal-to-Noise Ratio

CD sensitivity (mdeg/FS)	D.I.T. (sec)
1000	0.064 - 0.025
500	0.125 - 0.5
200	0.125 - 0.5
100	0.25 - 0.5
50	0.25 - 1.0
20	0.5 - 2.0
10	0.5 - 8.0
5	1.0 - 16.0
2, 1	4.0 - 16.0

**Note:** D.I.T. of 0.5 to 125 msec is used for high speed measurement using a stopped flow unit.

The above table also applies to step scan. In this case, the measurement time is determined by the sum of time of wavelength movement and wavelength stop time. If the D.I.T. is on order of seconds, the No. of integration will be dominant in the measurement time and the measurement time will be almost proportional to D.I.T.. Given that the wavelength interval of measurement wavelength section is W (nm) and the data interval is Step (nm), the following relation holds between total integration time and D.I.T..

$$\text{Total Integration Time} = (W/\text{Step} + 1) \times \text{D.I.T.}$$

(W/Step + 1) : Number of data points

<In time course measurement>

In time course measurement, select a D.I.T. suited to the CD signal change speed due to reaction, etc. In normal reaction, set it at 1/10 of half value period of D.I.T. or smaller. For example, if the half value period is 20 msec, a D.I.T. of 0.5 to 2 msec is appropriate. If the change is very slow, set the D.I.T. to 1 to 16 sec by considering the change speed and signal-to-noise ratio. When used as a monitor of HPLC, a D.I.T. of about one sec is suited.

(6) Band width and slit width

Usually, set the band width at 1.0 nm before measurement. Decrease it in the measurement of a sharp spectrum such as MCD, or increase it in the measurement by a micro cell, when the signal-to-noise ratio is low. When a long wavelength detector (400 to 1100 nm) is used, increase the band width and set the slit width to about 60  $\mu$ m to prevent the photomultiplier voltage (HT) from rising abnormally. However, see to it that HT does not become lower than 170 V.

**CAUTION:** As HT lowers below 170 V, increasing the slit width may damage the photomultiplier tube.

*Note: Most organic substances emit fluorescence. Therefore, measuring a sample having an absorbance of 2 or more at a band width of 2 nm or more may distort the spectrum. Also photolysis of sample can occur in the ultraviolet region. If the sample is susceptible to photolysis, reduce the band width to 0.5 nm or less according to its degree.*

(7) Sensitivity

Set a sample, move the wavelength and select an appropriate sensitivity from the maximum CD value while watching CD data. If the selected sensitivity is inappropriate and spectrum is too small or overflows, it can be redisplayed in an appropriate size after measurement. However, there is a limit to the analog signal that can be processed without being saturated to the selected sensitivity, as shown below.

When sensitivity is 1 to 100 mdeg/FS, normal up to  $\pm 100$  mdeg

When sensitivity is 200 to 1000 mdeg/FS, normal up to  $\pm 2000$  mdeg

If CD near  $\pm 200$  mdeg is measured with the full scale of 100 mdeg, data in that area may be distorted because noise components are contained in the analog signal. In such a case, set the full scale at 200 mdeg. In measuring CD, absorbance (Abs) is usually set at 2 or less. Therefore, a sample with low absorbance can be measured at a high concentration using a cell with long light path, allowing measurement with lower sensitivity than a sample with higher absorbance having similar ellipticity.

Since measurement with high sensitivity deteriorates the signal-to-noise ratio, minimize sensitivity by increasing sample concentration within the range Abs < 2 or by using a cell with long light path. (Refer to the manual for "CD/ORD measurement method").

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