

**JWJTC-515**

# **Temperature Control Program**

**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.

<p><i>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.</i></p>
--

## 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.***

## Notices

- (1) JASCO shall not be held liable, either directly or indirectly, for any consequential damage incurred as a result of product use.
- (2) Prohibitions on the use of JASCO software

Copying the software for purposes other than backup

Transfer or licensing the right to use software to a third party

Disclosure of confidential information regarding the software

Modification of the software

Use of the software on multiple workstations, network terminals, or by other methods  
(not applicable under a network licensing agreement concluded with JASCO)

- (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).

(C) JASCO Corporation, 2007. All rights reserved. Printed in JAPAN.

## Limited Warranty

Products sold by JASCO, unless otherwise specified, are warranted for a period of one year from the date of shipment to be free of defects in materials and workmanship. If any defects in the product are found during this warranty period, JASCO will repair or replace the defective part(s) or product free of charge.

THIS WARRANTY DOES NOT APPLY TO DEFECTS RESULTING FROM THE FOLLOWING:

- 1) IMPROPER OR INADEQUATE INSTALLATION
- 2) IMPROPER OR INADEQUATE OPERATION, MAINTENANCE, ADJUSTMENT OR CALIBRATION
- 3) UNAUTHORIZED MODIFICATION OR MISUSE
- 4) USE OF CONSUMABLE PARTS NOT SUPPLIED BY AN AUTHORIZED JASCO DISTRIBUTOR
- 5) CORROSION DUE TO THE USE OF IMPROPER SOLVENTS, SAMPLES, OR DUE TO SURROUNDING GASES
- 6) ACCIDENTS BEYOND JASCO'S CONTROL, INCLUDING NATURAL DISASTERS
- 7) CONSUMABLES AND PARTS OF WHICH THE WARRANTY PERIOD IS OTHERWISE SPECIFIED.

THE WARRANTY FOR ALL PARTS SUPPLIED AND REPAIRS PROVIDED UNDER THIS WARRANTY EXPIRES ON THE WARRANTY EXPIRATION DATE OF THE ORIGINAL PRODUCT. FOR INQUIRIES CONCERNING REPAIR SERVICE, CONTACT YOUR JASCO DISTRIBUTOR AFTER CONFIRMING THE MODEL NAME AND SERIAL NUMBER OF YOUR INSTRUMENT.

JASCO Corporation  
2967-5, Ishikawa-machi, Hachioji-shi  
Tokyo 192-8537,  
JAPAN



# 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>
1.1 How to use this Manual .....	1
1.2 Overview of the JASCO Temperature Controlling Program .....	2
1.3 Notation Used in this Manual .....	2
1.4 Program Window .....	3
<b>2. Installing Accessories</b> .....	<b>5</b>
2.1 Installing the [Temperature Control] program .....	5
2.2 Registration of the Peltier Accessory .....	8
2.3 Registration in the Program Window .....	10
<b>3. [Variable Temperature Measurement] Menu Reference</b> .....	<b>12</b>
3.1 [Measurement] Menu .....	14
3.1.1 [Parameters...] .....	14
3.1.1.1 [Temperature] Dialog Box .....	14
3.1.1.2 [General] Dialog Box .....	15
3.1.1.3 [Control] Dialog Box .....	17
3.1.1.4 [Information] Dialog Box .....	18
3.1.1.5 [Data] Dialog Box .....	19
3.1.1.6 Common function .....	20
3.2 [Control] Menu .....	21
3.2.1 [Select Accessory...] .....	21
3.2.2 [Move Wavelength...] .....	21
3.2.3 [CD Detector...] .....	22
3.2.4 [Light Source...] .....	22
3.2.5 [Shutter...] .....	23
3.2.6 [ORD-M Zero Clear] .....	23
<b>4. Introduction to [Variable Temperature] Program</b> .....	<b>24</b>
4.1 Operation Overview .....	24
4.2 Measuring, Saving and Printing Data .....	24
4.2.1 Sample Preparation .....	24
4.2.2 Starting the Temperature Variable Measurement Program .....	25
4.2.3 Setting Parameters .....	26
4.2.4 Setting Sample and Measurement .....	29
4.2.5 Saving Data and Parameters .....	32

4.2.5.1 Saving Parameters .....	32
4.2.5.2 Saving Baseline Data.....	33
4.2.5.3 Saving Sample Data .....	33
4.2.6 Sending Data to [Spectra Analysis] .....	34
4.2.7 Printing Spectrum .....	35
<b>5. [Temperature Interval Scan Measurement] Menu Reference .....</b>	<b>36</b>
<b>5.1 [Measurement] Menu .....</b>	<b>38</b>
5.1.1 [Parameters...].....	38
5.1.1.1 [Temperature] Dialog Box .....	38
5.1.1.2 [General] Dialog Box .....	39
5.1.1.3 [Control] Dialog Box.....	42
5.1.1.4 [Information] Dialog Box.....	42
5.1.1.5 [Data] Dialog Box .....	43
5.1.1.6 Common function.....	44
5.1.2 [Monitor Parameters...].....	44
<b>5.2 [Control] Menu.....</b>	<b>45</b>
5.2.1 [Select Accessory...] .....	45
5.2.2 [Move Wavelength...] .....	45
5.2.3 [CD Detector...] .....	46
5.2.4 [Light Source...].....	46
5.2.5 [Shutter...].....	47
5.2.6 [ORD-M Zero Clear].....	47
<b>6. Introduction to [Temperature Interval Measurement] Program .....</b>	<b>48</b>
<b>6.1 Operation Overview.....</b>	<b>48</b>
<b>6.2 Measuring, Saving and Printing Data.....</b>	<b>49</b>
6.2.1 Sample Preparation.....	49
6.2.2 Starting the Temperature Variable Measurement Program .....	49
6.2.3 Setting Parameters .....	50
6.2.4 Setting Sample and Measurement .....	54
6.2.5 Saving Data and Parameters .....	56
6.2.5.1 Saving Parameters .....	56
6.2.5.2 Saving Sample Data .....	57
6.2.6 Sending Data to [Spectra Analysis] .....	57
6.2.7 Printing Spectrum .....	58

# 1. General

## 1.1 How to use this Manual

This manual is for the JASCO temperature control program that runs on the Spectra Manager ver 2.0 program. In this manual, Microsoft Windows 2000/XP Professional Edition is referred to as “Windows” and a personal computer as “PC”.

It is made up of six sections, including this section. Each section contains following information.

1. Introduction  
Describes how to use this manual and contains overviews of the [Temperature Control] programs, *i.e.*, [Peltier Control], [Variable Temperature Measurement] and [Temperature Interval Scan Measurement] programs along with the menus for these programs. Read this section first.
2. Setting accessory  
Contains the procedure for installing the [Temperature Control] programs, registering the Peltier accessory in [Spectra Manager], setting a communication port on a PC and in the [Variable Temperature Measurement] program and/or [Temperature Interval Scan Measurement] program. This procedure is needed when controlling the Peltier accessory automatically.
3. [Variable Temperature Measurement] menu reference  
Menu reference for the [Variable Temperature Measurement] program. Read relevant sections as and when required.
4. Practical use of [Variable Temperature Measurement]  
Contains procedures for starting up this program, measuring samples, saving the data obtained onto disk and printing out the results using the [Variable Temperature Measurement] program.
5. [Temperature Interval Scan Measurement] menu reference  
Menu reference for the [Temperature Interval Scan Measurement] program. Read relevant section as and when required.
6. Practical use of [Temperature Interval Scan Measurement] program  
Contains procedures for starting up this program, measuring samples, saving the data obtained onto disk and printing out the results using the [Temperature Interval Scan Measurement] program.



## 1.2 Overview of the JASCO Temperature Controlling Program

There are three kinds temperature controlling programs, *i.e.*, the [Peltier Controlling] program, the [Variable Temperature Measurement] program and the [Temperature Interval Scan Measurement] program. The [Peltier Controlling] program is used for controlling the Peltier automatically. The [Variable Temperature Measurement] program is used for measuring the CD change at a certain wavelength as function of temperature change, while the [Temperature Interval Scan Measurement] program is for measuring the CD change at a certain wavelength and CD spectra at several given temperatures.

**Note(1):** The Peltier-type temperature control system can be used with a single cell holder but not with a six-cell changer.

**Note(2):** The temperature controlling program can only be used for the Peltier control system, and not for bath circulator-type controlling systems.

**Note(3):** The temperature controlling program runs from the Spectra Manager ver 2.0 program which runs on Microsoft Windows 2000/XP Professional Edition.

## 1.3 Notation Used in this Manual

To aid comprehension, the following notation is used throughout this manual.

### General Notation

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

### Keyboard Operations

Notation	Meaning
<b>Shift CTRL</b>	The key is enclosed by a square and shown in boldface.
<b>Alt, F</b>	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.
<b>Shift + →</b>	Keys that are pressed simultaneously are separated by a "plus" sign. In the example shown on the left, press the “→” key while holding down the “Shift” key.

### Mouse Operations

Notation	Meaning
<b>Point</b>	Move the mouse pointer to the specified item.
<b>Click</b>	Quickly press and release the mouse button.
<b>Double-click</b>	Click the mouse button twice in rapid succession.
<b>Drag</b>	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) Temperature Controlling Program Window

Figure 1.1 depicts the names of features in the program window of the [Variable Temperature Measurement] program (the [Temperature Interval Scan Measurement] program is the same). Figure 1.2 is displayed by clicking the [Variable Temperature Measurement] menu of Figure 1.2.

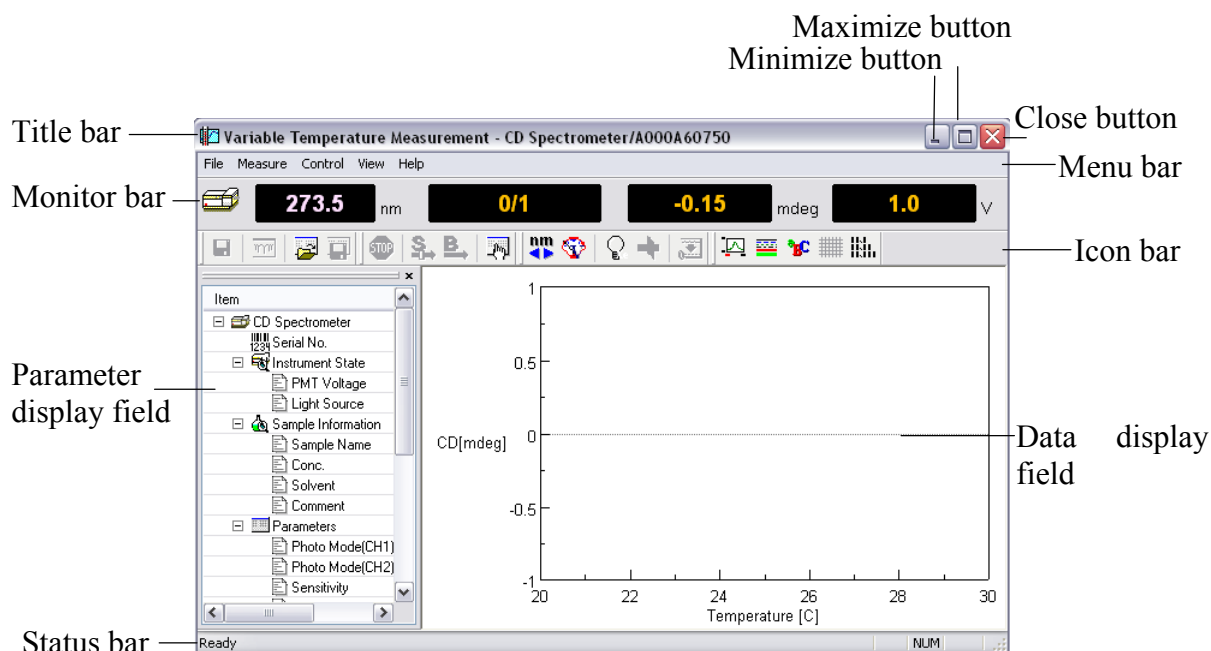


Figure 1.1 [Variable Temperature] window

**Note:** Figure 1.1 depicts only one channel of data, but this program can display up to a maximum of four channels of data simultaneously when measurement starts.

Name	Function
Title bar	Displays the program name. The appearance of the title bar of the active window (the window in which the operator is working) differs from that of inactive windows in both color and brightness.
Menu bar	Displays the names of the menus that can be used. Each menu contains commands (operations) that can be 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 Figure. 1.2). The left side of the window shows the installed programs, which are the J-800 [Spectra Analysis], the J-800 standard program and the [Thermo Controlling] program. From this window it is possible to control the operation of the spectrometer and program, transfer data files into [Spectra Analysis], open graphs and information as a data file, display the directory of the data file and open the [Administrative Tools].

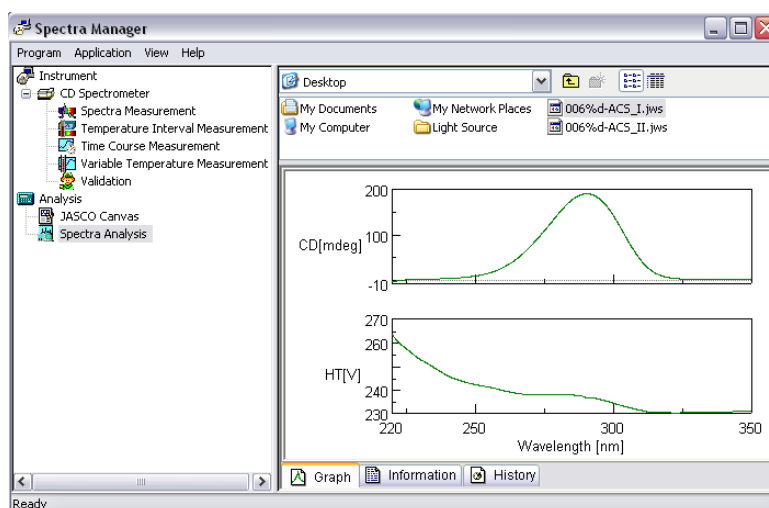


Figure 1.2 [Spectra Manager] window

## (3) [Spectra Analysis] window

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

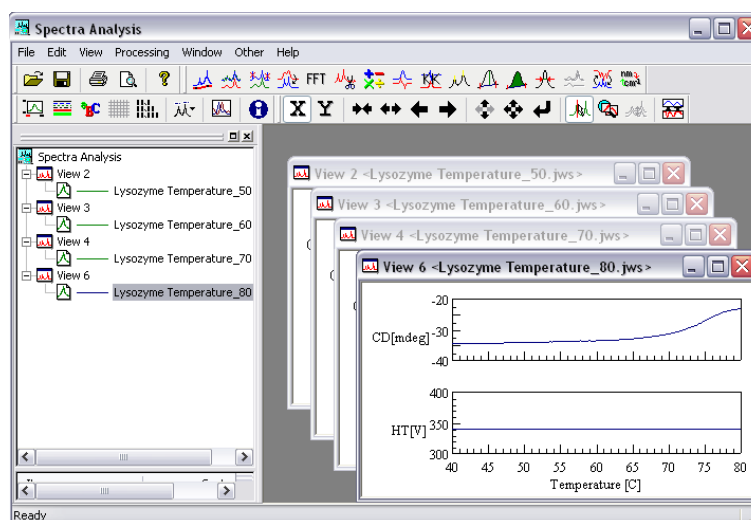


Figure 1.3 [Spectra Analysis] window

**Note:** Refer to the “Spectrum Analysis Operation Manual” for more information.

## 2. Installing Accessories

This section contains the procedures for installing the [Temperature Control] program, registering the Peltier accessory and setting the communication (COM) port and the paths to the programs.

**Note:** Installing [Temperature Control] program is done after installing the Spectra Manager Var.2.registering

**Note:** Refer to the “J-800 Series Operation Manual” for how to install [Spectra Manager], [Spectral Analysis] and standard programs of the J-800 series and registering the spectrometer and measurement programs .

### 2.1 Installing the [Temperature Control] program

There are two kinds of folders. The [Variable Temperature Measurement] and [Temperature Interval Scan Measurement] programs are located in the “CDTempCtPrg” folder, while the [Peltier Controlling] program is located in the “ETCEHCPSCThermoDrv” folder.

**Note:** The programs in the “ETCEHCPSCThermoDrv” folder should be installed first.

Select the [Administrative Tools] - [Program] menu of the [Spectra Manager] window. The following window appears.

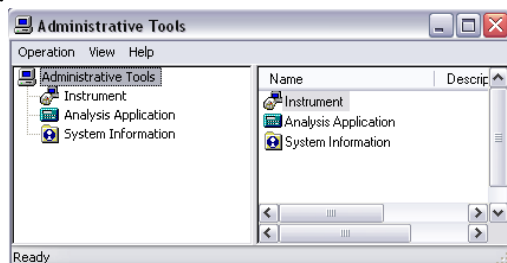


Figure 2.1 [Administrative Tools] window

- (1) Select the [Operation] - [Install...] menu.
- (2) Click the <Browse...> button and select the “ETCEHCPSCThermoDrv” folder by clicking the folder. The program is recognized and the name “ETCEHCPSCThermoDrv” appears in the [Spectra Manager Setup] screen (See Figure. 2.2).

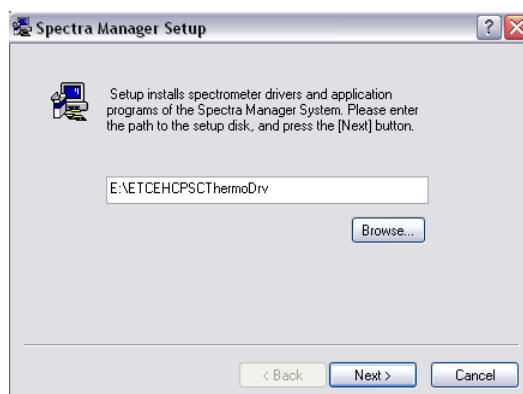


Figure 2.2 Data directory input screen

**Note(1):** The target program should not be located on the desktop. A floppy disk, removable disk, or local disk drive C: are the most suitable locations.

**Note(2):** Refer to the “Windows Manual” for how to use “Explorer”.

- (3) Click the <Next> button. The recognized program appears as shown in Figure. 2.3.

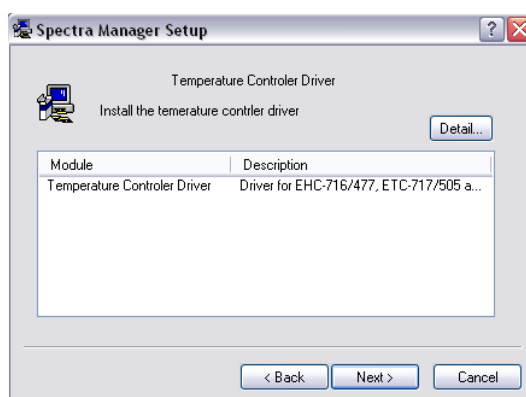


Figure 2.3 Recognized [Temperature Control] program

- (4) Click the <Next> button. The program is installed and the following screen appears when installation has finished.

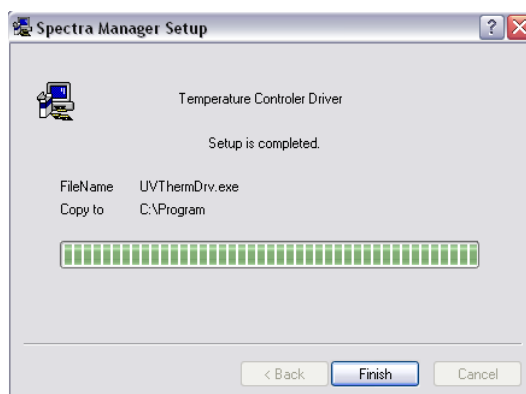


Figure 2.4 The dialog box when installation has been completed

- (5) Click the <Finish> button.

The installation of the contents of the “CDTempCtPrg” folder, *i.e.*, the [Variable Temperature Measurement] and [Temperature Interval Scan Measurement] programs follows the same procedure given in steps (1) – (5).

- (6) Install the contents of the “CDTempCtPrg” folder.

**Note:** Clicking the <Back> and <Cancel> buttons reverts to the previous screen and the [Administrative Tools] window, respectively.

- (7) Close the [Administrative Tools] and [Spectra Manager] windows and reopen the [Spectra Manager] window. The [Variable Temperature Measurement] and [Temperature Interval Scan Measurement] menus are updated as shown in Figure. 2.5.

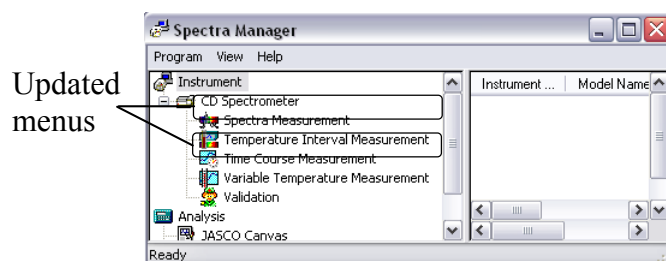


Figure 2.5 [Spectra Manager] window after installation

**Note:** [Peltier Control] Program does not appear in the [Spectra Manager] window.

## 2.2 Registration of the Peltier Accessory

Registration of the Peltier accessory is done from the [Administrative Tools] window. Open the [Administrative Tools] window of Figure. 2.1 and to display the [CD Spectrometer] menu shown in Figure. 2.6 (the [CD Spectrometer] menu is in the [Instrument] menu of the [Administrative Tools] window).

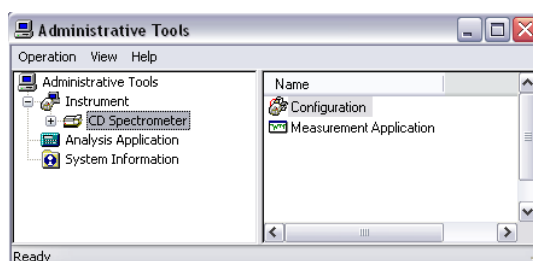


Figure 2.6 [Administrative Tools] window

- (1) Select [Properties...] - [Operation] menu after clicking the [CD Spectrometer] menu. The [Properties] screen appears.
- (2) Click the [Cell Unit] tab in the [Properties] screen. The following window appears.

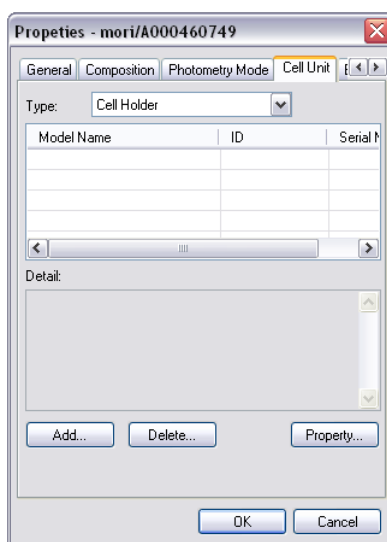


Figure 2.7 [Properties] screen when the <Cell Unit> tab is selected (dialog title spelling)

- (3) Select the [Temperature Controller] menu by clicking the arrow on the extreme right of the <Type> box.
- (4) Check the <Add...> button of Figure. 2.7. The following screen appears.

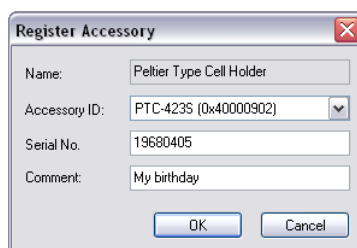


Figure 2.8 [Register Accessory] screen

- (5) Select “PTC-423S” by clicking the arrow on the extreme right of the <Accessory ID> box.
- (6) Enter the serial No. in the <Serial No.> boxes. Write a comment if necessary.

**Note:** The <Serial No.> should be entered correctly. If entered incorrectly, the measurement programs will not work well.

- (7) Click the <OK> button. The screen of Figure. 2.7 becomes as follows when the accessory “PTC-423S” has been registered correctly.

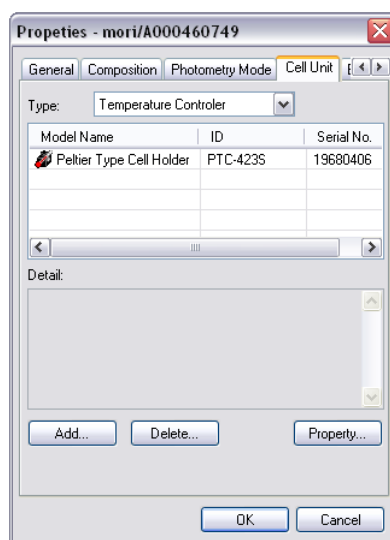


Figure 2.9 [Administrative Tools] screen after a successful installation

- (8) Click the <Property...> button. The following dialog box appears.

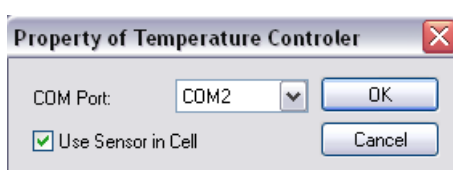


Figure 2.10 [Property of Temperature Controller] dialog box

**Note (1):** The COM port for the Peltier accessory must be COM2 if that for the spectrometer is set to COM1.

**Note (2):** The COM port setting for the spectrometer can be done from the [Properties] screen which appears when the <General> tab is clicked. Refer to the “J-800 Series Operation Manual” for more information.

- (9) Click the <OK> button of Figure. 10. It returns to the screen shown in Figure. 2.9.
- (10) Click the <OK> button of Figure. 2.9. It returns to the [Administrative Tools] window of Figure. 2.6.
- (11) The registration procedure is completed by closing the [Administrative Tools] window of Figure. 2.6.



## 2.3 Registration in the Program Window

Register the Peltier accessory in the [Variable Temperature Measurement] or [Temperature Interval Scan Measurement] program. Registration is performed using [Select Accessory]. Open the desired program by clicking the menu in the [Spectra Manager] window.

**Note (1):** Ensure the power supply of the spectrometer and the Peltier accessory are turned ON, the PC is started up and the COM ports are set appropriately. Refer to the “J-800 Series Operation Manual” for more information regarding starting up the spectrometer and setting the COM port of the spectrometer. Refer also to Section 2.2 for setting the COM port for the Peltier accessory.

**Note (2) :** The registration must be performed whenever the measurement programs are run. Otherwise, the accessory cannot be controlled.

**Note (3):** If the [Select Accessory...] menu does not appear in the [Control] menu, check whether the accessory has been registered (refer to Section 2.2)

- (1) Select [Select Accessory...] in the measurement window. The following screen appears.

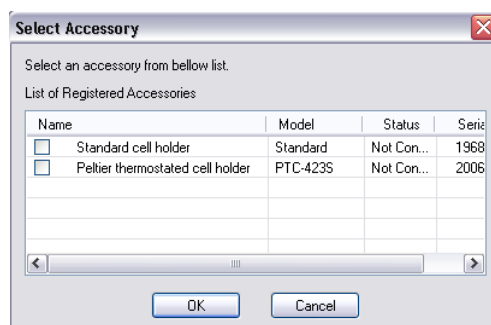


Figure 2.11 [Select Accessory] screen

- (2) Click the <OK> button after inserting a check mark for the Peltier thermostated cell holder (PTC-423S). The following dialog box appears.

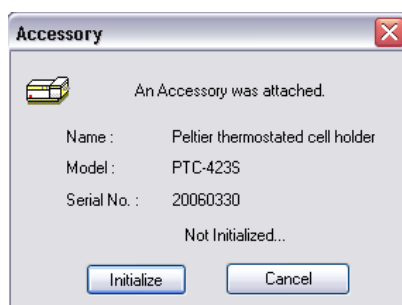


Figure 2.12 [Accessory] dialog box

- (3) Click the <OK> button. Setting the path has been completed and the following picture is displayed on the left side of the measurement program.

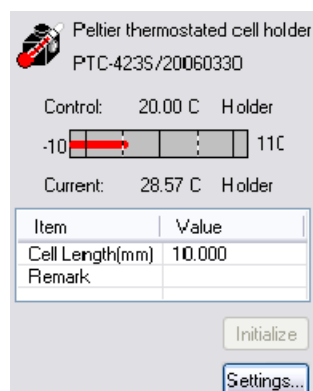


Figure 2.13 [Accessory] dialog box

**Note:** Clicking the <Cancel> button reverts to the measurement program window.

### 3. [Variable Temperature Measurement] Menu Reference

Start the [Variable Temperature Measurement] program. Start the following window by clicking the [Variable Temperature Measurement] menu that appears in the [Spectra Manager] window.

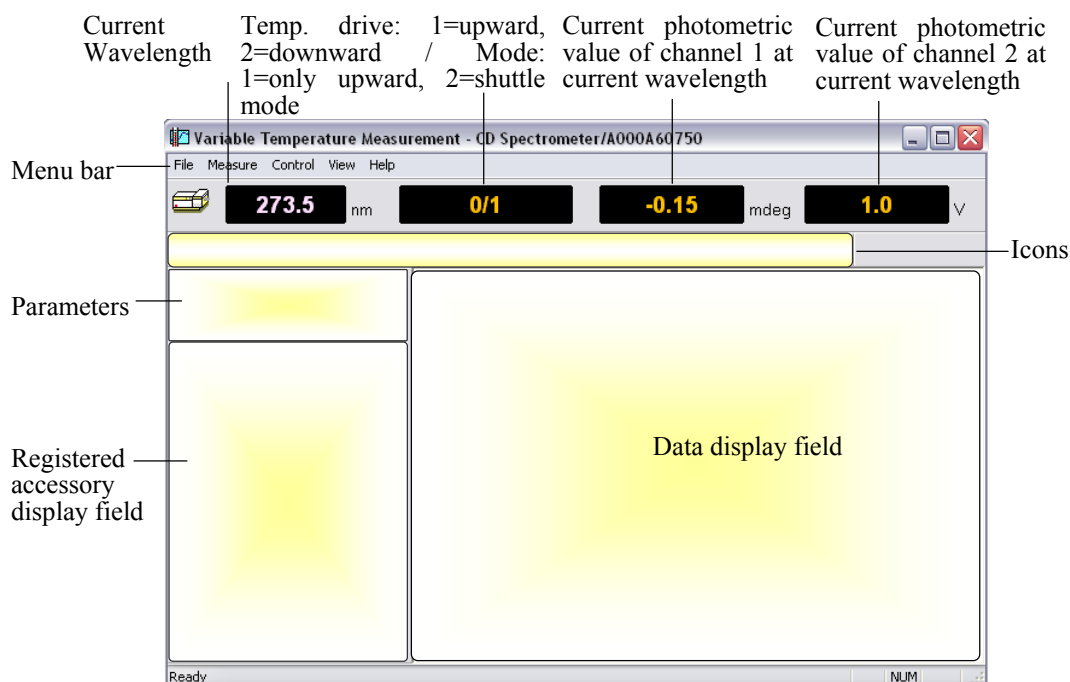


Figure 3.1 [Variable Temperature Measurement] window

**Note (1):** Figure. 1.1 shows one channel of data, but this program can display a maximum of four channels of data simultaneously when measurement starts.

**Note (2):** Refer to Section 2.2 and Section 2.3 for registration of the Peltier accessory.

**Note (3):** Refer to the “J-800 Series Operation Manual” for how to start the [Spectra Manager] program.

#### [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 files which are .cdbtv format files.  |
| [Save Baseline...]   | Saves [Baseline] data to disk as .cdbtv format files.   |
| [Open Parameters...] | Opens temperature variable measurement parameters which are set in the [Parameter Settings] dialog box. The file format is .cdtv. |
| [Save Parameters...] | Saves measurement parameters as a .cdtv format file.  |
| [Exit]               | Exits the [Spectra Measurement] window.   |



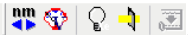

## **[Measure] menu**

[Parameters...]	Sets measurement parameters, control portions of Peltier (sample cell holder or sample cell), monitoring sensor portion (sample cell holder or sample cell), toggles [Baseline] or [Blank] measurement and auto-shutter control ON/OFF, edits comments and saves and loads measurement parameters and data.
[Sample...]	Starts measurement of sample.
[Baseline]	Starts a [Baseline] or [Blank] measurement.
[Cancel]	Stops blank and sample measurement.

## **[Control] menu**

[Move Wavelength...]	Moves the current wavelength to the desired value.
[CD Detector...]	Sets the sensitivity of the detector (CD/ORD/LD/UV).
[Light Source...]	Toggles 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).
[Select Accessory...]	Registers compatible accessories.
[PTC-423S]	Sets temperature and the portion controlling and monitoring the temperature of the sample cell holder or sample cell. This menu appears when Peltier is registered.

## **[View] menu**

[Select Graph...]	Selects the desired channel No. (default is channel 1).
[Overlay]	Overlays graphs.
[Scale...]	Sets the minimum and maximum values for the vertical and/or horizontal axes/axis.
[Pattern...]	Sets the color, style and width of lines (spectra).
[Font...]	Sets the font type for the axes values and/or unit(s).
[Grid...]	Displays or hides grid.
[Style...]	Sets the scale interval.
[Information Bar]	Displays or hides parameters such as those shown in Figure. 4.1.
[Toolbar...]	Displays or hides the toolbars shown in Figure. 4.1.
[File]	Displays or hides the [File] toolbar:  .
[Measure]	Displays or hides the [Measure] toolbar:  .
[Control]	Displays or hides the [Control] toolbar:  .
[View]	Displays or hides the [View] toolbar:  .
[Status Bar...]	Displays or hides the status bar of Figure. 3.1.
[Temp. Monitor Bar]	Displays holder temp., cell temp., ideal temp. and/or given temp. at each measurement point.
[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 information.

## 3.1 [Measurement] Menu

### 3.1.1 [Parameters...]

Sets the measurement parameters, control portions of Peltier (sample cell holder or sample cell), monitoring sensor portion (sample cell holder or sample cell), turns [Baseline] or [Blank] measurement and auto-shutter control ON/OFF, edits comments and saves and loads measurement parameters and data. The parameters dialog box is made up of five dialog boxes: [Temperature], [General], [Control], [Information] and [Data]. They can be changed by clicking the appropriate tab at the top of the box.

#### 3.1.1.1 [Temperature] Dialog Box

Sets the measurement parameters for temperature.

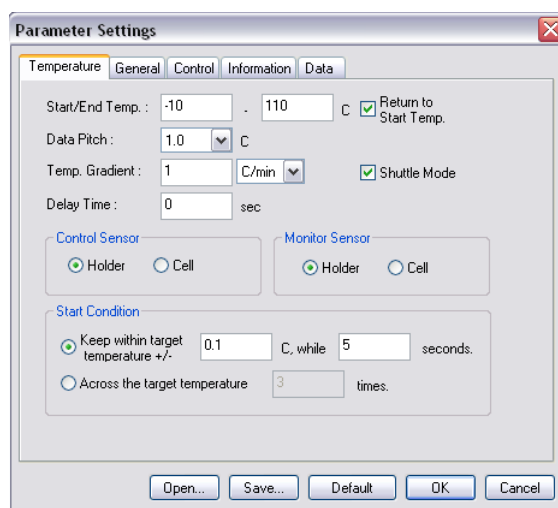


Figure 3.2 [Temperature] dialog box

#### Menu

- |                        |   |
|------------------------|---|
| [Start/End Temp]       | Sets the initial temperature (left box) and the final temperature (right box). Temperature increases during course of measurement. Temperature range: -10.0°C – 110.0°C. Temperature can be specified to the first decimal place.                                   |
| [Data Pitch]           | Selects the data acquisition interval by clicking the arrow on the extreme right of the [Data Pitch] box. Range: 0.1°C – 10.0°C.  |
| [Temp. Gradient]       | Sets the temperature increasing and decreasing rate (temperature/time). The units °C/minute or °C/hour can be selected by clicking the arrow on the extreme right of the box. Range: 0 – 10°C/min and 0 – 600°C/hr. It can be specified to the sixth decimal place. |
| [Delay Time]           | Sets the delay time, which is the time before the measurement commences after the target temperature has been reached. Range: 0 sec – 3600 sec, where only integers can be entered.   |
| [Return to Start Temp] | Returns to the [Start] temperature when the measurement has finished. Put a check mark in the box if required.  |
| [Shuttle mode]         | Performs a measurement by decreasing the temperature after completing a measurement during which the temperature is increased. Put a check mark in the box if required.   |
| [Control Sensor]       | Selects the sensor, either surrounding the sample cell [Holder] or in the   |

- inner cell [Cell], for controlling the temperature. Select either [Holder] or [Cell] by clicking one of these options.
- [Monitor Sensor] Selects the sensor, either surrounding the sample cell [Holder] or in the inner cell [Cell], for monitoring temperature. Select either [Holder] or [Cell] by clicking one of these options.
- [Start Condition] Two criteria for attaining the target temperatures are presented.  
CASE I: Determines the temperature range (°C) and the time (seconds) after the temperature enters the specified temperature range. The ranges are 0 – 10°C and 0 – 60 sec, respectively. They can be specified to the first decimal place and as an integer, respectively.  
CASE II: Determines the number of crossing points (times) with the target temperature. Range: 0 – 10 times.

### 3.1.1.2 [General] Dialog Box

Sets other measurement parameters besides the temperature.

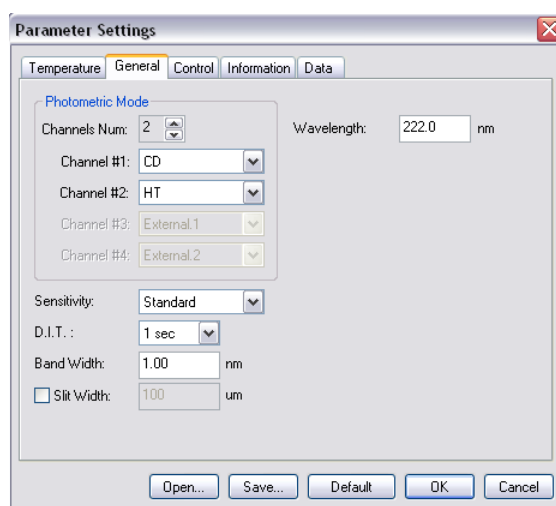


Figure 3.3 [General] dialog box

### Menu

- [Channel Num] Maximum of four channels. Four types of data can be acquired simultaneously.
- [Channel #1] The selectable range varies with the optional accessory used.  
CD: Circular dichroism signal, which is given by  $\sim AC/DC$  with 50 kHz.  
CD/DC: This is the same as the 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 the LD accessory is installed): Linear dichroism signal, which is given by  $\sim AC/DC$  with 100 kHz.  
ORD-M (when the 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 the ORD-E accessory is installed): Optical rotational dispersion which is controlled electronically.

UV (single): DC signal.

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

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

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

FDCD/DC (when the 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 located on the rear panel of the amplifier) and Abs.
[Channel #4]	For external input signals (from the "EXT 2" terminal located on the rear panel of the amplifier).
[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)], designates 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 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]	Sets the wavelength for measurement. Range: 163 – 1100 nm; it can be specified to the first decimal place.

<b>CAUTION:</b> 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.
---

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

<b>Note (2):</b> If the entered value exceeds the limits for that parameter, an error message will be displayed.
--

<b>Note (3):</b> The acceptable range of values for the [Band Width] and [Wavelength] are not the same as those for the instrument. Refer to "J-815 Hardware Manual" for its specification.
---

<b>Note (4):</b> 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 thermostated cell holder or a pH meter.
---

### 3.1.1.3 [Control] Dialog Box

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

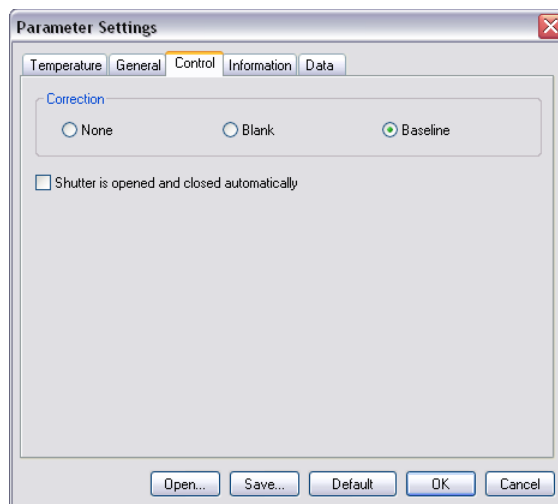


Figure 3.4 [Control] dialog box

#### Menu

[Blank]	Performs correction data at room temperature using one set of data.
[Baseline]	This is the same condition with [Sample] measurement.
[None]	Turns the correction OFF.
[Auto shutter]	Automatically opens the shutter just before measurement starts. Put a check mark if this function is required.

**Note (1):** If baseline correction is performed, the spectra acquired has the baseline subtracted from it.

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

**Note (3):** Auto-shutter drive works immediately before and immediately after the measurement.

The availability/unavailability of baseline correction for different menus are listed as follows.



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

**Note:** The availability of baseline correction is indicated on the monitor bar in the [Spectra Measurement] window: if it is available, the figures in the [Spectra Measurement] window are displayed in white after baseline measurement has been performed.

#### 3.1.1.4 [Information] Dialog Box

Figure 3.5 [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 number of characters that can be entered. The concentration unit, mol/l, mmol/l,  $\mu$ mol/l, nmol/l, w/v%, ppm and ppb can be selected.

### 3.1.1.5 [Data] Dialog Box

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

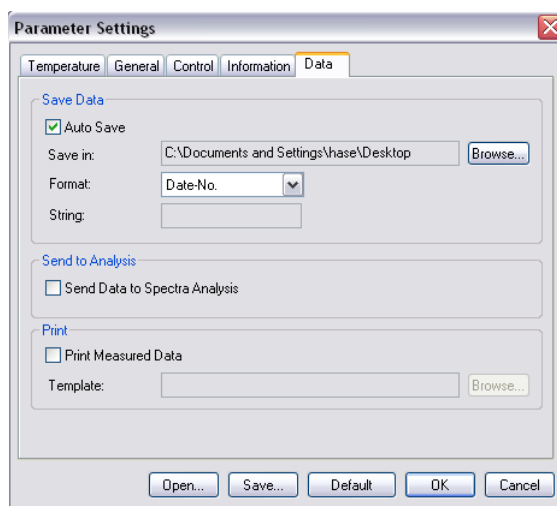


Figure 3.6 [Data] dialog box

[Save Data]

Sets whether acquired spectrum is to be saved automatically or not. If a check mark is inserted in the [Auto Save] box, the filename and directory where the spectrum is to be saved should be entered in the dialog box. This function is useful for repeated measurements.

[Save in]

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

[Format]

Date-No.	Displays the date and file number
Sample-No.	Displays the sample name and file number, 1, 2, 3...
Comment-No.	Displays the 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]

Enter the filename of your choice, 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 the filename and directory where the spectrum is to be saved in the dialog box. This is useful for repeated measurements.

[Send data to Spectra Analysis]

Automatically transfers data to the [Spectra Analysis] program.

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

<b>Note (2):</b> When using [Send data to Spectra Analysis] mode with several cycle times, multiple sets of data are sent to [Spectra Analysis] window.
---

### 3.1.1.6 Common function

The following buttons work in all screens, [Temperature], [General], [control], [information] and [Data].

<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 parameters from disk. Clicking this button displays the [Open] dialog box. Selecting baseline data here and clicking the <Open> button loads the baseline data into the memory. Opens data in the .cdtv format.
<Save>	Saves the parameters in the .cdtv format.
<Default>	Reverts to the default parameters.

## 3.2 [Control] Menu

### 3.2.1 [Select Accessory...]

**Note:** Whenever using a temperature controller, the Peltier accessory should be registered. Otherwise, the temperature cannot be controlled.

Refer to Section 2.3 for details. [PTC-423S] are displayed in the [Control] menu after registering the Peltier accessory. Select [PTC-423S] and the following dialog box is displayed.

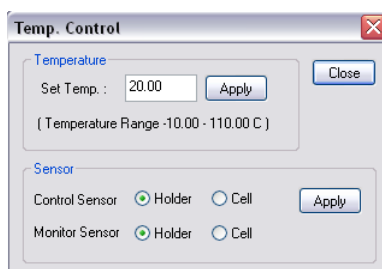


Figure 3.7 [Temp. Control] dialog box

[Set Temp.]	Sets the temperature. Range: -10 to 110°C.
<Apply>	Applies the set temperature.
[Control Sensor]	Sets area in which temperature is controlled. <Holder>: sample cell holder, <Cell>: sample cell.
[Monitor Sensor]	Sets sensor for monitoring temperature.
<Apply>	Applies the settings.
<Close>	Closes the dialog box of Figure. 5.8.

**Note:** Whenever using a temperature controller, the Peltier accessory should be registered. Otherwise, temperature cannot be controlled.

### 3.2.2 [Move Wavelength...]

Moves the wavelength to the desired value.

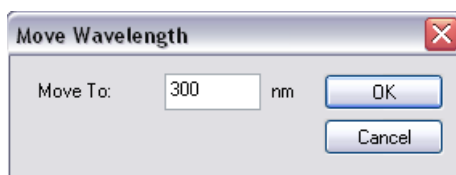


Figure 3.8 [Move Wavelength] dialog box

[Wavelength]	Text box for input. Range: 165 nm to 1100 nm.
<OK>	Moves the wavelength to the set wavelength.
<Cancel>	Closes the dialog box without changing the previous wavelength setting.

### 3.2.3 [CD Detector...]

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

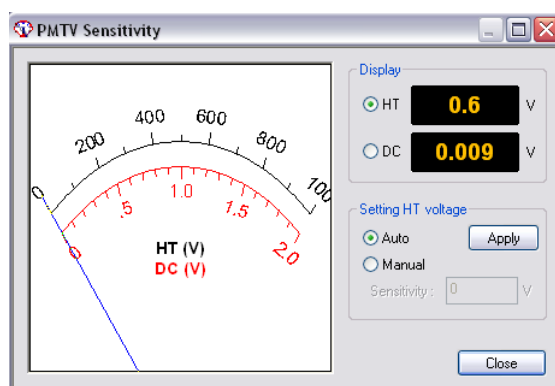


Figure 3.9 [PMTV Sensitivity] dialog box

[Display]	Changes the meter indication (displayed on the right side of Figure 3.9) at the right of [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] using the 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 is not displayed in the [Spectra Measurement] window and then it cannot be obtained.

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

### 3.2.4 [Light Source...]

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



Figure 3.10 [Light Source Control] dialog box

[Xe Lamp] Turns the lamp ON/OFF. The icon is toggled by clicking it.



Icon indicating that the lamp is on.



Icon indicating that the lamp is off.

The operating time of the lamp is displayed in Figure. 3.10. (0.0 hour in this case)

<OK> Turns the lamp ON/OFF.

<Cancel> Closes the dialog box without changing anything.

**Note:** If the light source does not come on, try to turn it on several times. If you still have problems, contact your local JASCO distributor.

### 3.2.5 [Shutter...]

Opens or closes the shutter. Only effective for an instrument having a shutter.

This instrument uses a high output xenon lamp as the light source. It irradiates a sample with high intensity ultraviolet radiation. When measuring a sample that is susceptible to photolysis, minimize the irradiation time or narrow the slit width to reduce the beam intensity. For such samples, open the shutter only during measurement by using this function.

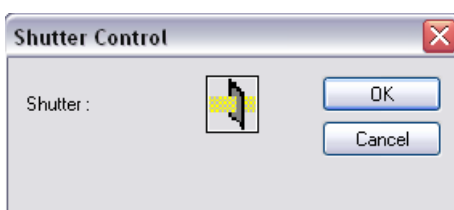


Figure 3.11 [Shutter Control] dialog box

[Shutter] Turn the shutter ON/OFF. The icon is toggled by clicking it.



Icon indicating that shutter is open.



Icon indicating that shutter is closed.

<OK> The shutter opens or closes.

<Cancel> Closes the dialog box without changing anything.

**Note (1):** Closing the shutters zeroes the HT voltage. Confirm this in the [CD Detector...] dialog box (Figure. 3.9) if necessary.

**Note (2):** When the spectrometer is turned ON, the shutter automatically opens. Check the front LED to see if the shutter is ON/OFF in this case.

### 3.2.6 [ORD-M Zero Clear]

This is effective only when ORD-M is installed.

## 4. Introduction to [Variable Temperature] Program

This section contains the procedures for starting up the [Variable Temperature Measurement] program, measuring the sample, saving the measured data on disk and printing out the result to familiarize the operator with operation.

**Note (1):** Refer to the instruction manuals for accessories on how to start the spectropolarimeter and accessories and to register the accessories. Here, the description starts from the startup of [Variable Temperature Measurement] program from the [Spectra Manager] program.

**Note (2):** Here, it is assumed that the Peltier-type single cell holder has been connected.

### 4.1 Operation Overview

Starting spectrometer	Refer to "Hardware manual".
↓	
Sample preparation	See "4.2.1".
↓	
Starting Temperature Variable Measurement Program	See "4.2.2".
↓	
Registering Accessories on [Variable Temperature Measurement]	See to "2.3".
Setting Parameters	See "4.2.3".
↓	
Setting Sample and Measurement	See "4.2.4".
↓	
Saving Data and Parameters	See "4.2.5".
↓	
Sending Data to [Spectra Analysis]	See "4.2.6".
↓	
Printing Spectrum	See "4.2.7".

### 4.2 Measuring, Saving and Printing Data

How to measure, save and print data using 0.0074 mol/l Lysozyme (Lyz) in water solution with 10 mM phosphate buffer is explained.

#### 4.2.1 Sample Preparation

Prepare about 1 mg Lyz and put it into 10 ml of 10 mM phosphate buffer solvent. Put the prepared sample into a 0.1 cm cell.

**Note (1):** The Lyz solution should be prepared immediately prior to performing the measurement.

### 4.2.2 Starting the Temperature Variable Measurement Program

**Note:** Ensure the power supplies of the spectrometer and the Peltier accessory are turned ON, the COM ports are set appropriately and the accessory is registered in [Administrative Tools]. Refer also to Section 2.2 for more information.

- (1) Double-click the [Temperature Variable Measurement] menu in the [Spectra Manager] window. The window shown in Figure. 1.1 appears.
- (2) Register the Peltier accessory following the procedure described in Section 2.3. The [Temperature Variable Measurement] window appears as shown below (it is similar to Figure. 3.1).

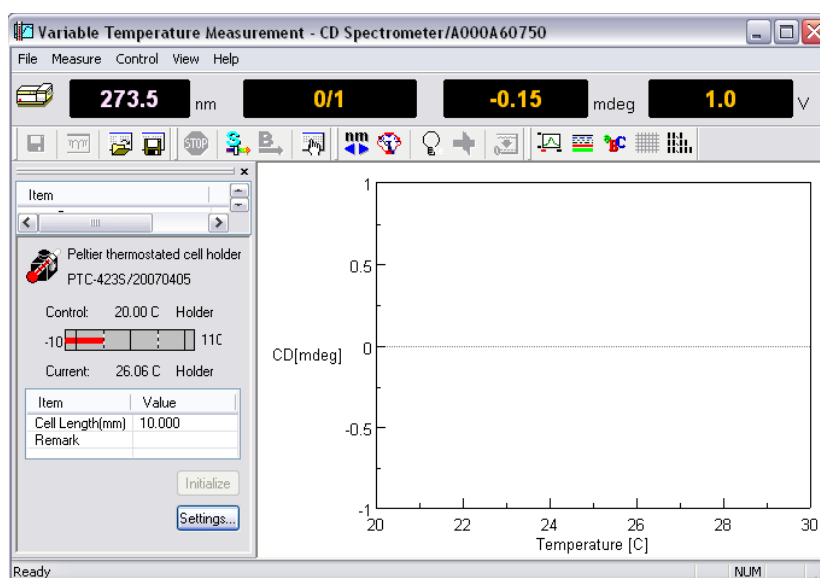


Figure 4.1 [Temperature Variable Measurement] window

**Note:** Ensure the power supplies of the spectrometer and the Peltier accessory are turned ON, the COM ports are set appropriately and the accessory is registered in [Administrative Tools]. Refer also to Section 2.2 for more information.

- (3) Select [PTC-423S] from the [Control] menu or click the <Settings...> button of Figure. 4.1. The following dialog box appears.

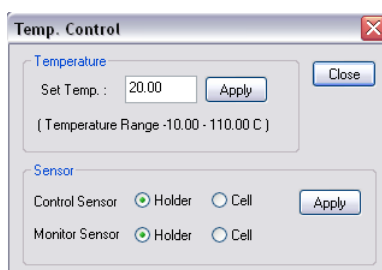


Figure 4.2 [Temp. Control] dialog box

- (4) Enter the desired temperature into the text boxes and click the <Apply> button. To input a value for a parameter click its text box. A cursor appears in the text box, waiting for input. Delete unnecessary numerals and input the desired value using the numeric keys.




- (5) Set the desired menus for [Control Sensor] and [Monitor Sensor], which are the areas for controlling temperature and monitoring the temperature, respectively.
- (6) Clicking the <Close> button registers the temperature.

**Note (1):** After clicking the <Close> button, the “Stop” sign in the front panel of Peltier accessory becomes a “Start” sign.

**Note (2):** Refer to the “PTC-423 Manual” for how to use the accessory safely and correctly.

### 4.2.3 Setting Parameters

- (1) Click the  icon or select [Parameters...] from the [Measure] menu of Figure. 4.1. The following dialog box appears. The parameters setting dialog box is composed of the [Temperature], [General], [Control], [Information] and [Data] dialog boxes. Clicking a tab at the top of the dialog box changes the dialog box. Refer to Section 3.1.1 for descriptions of these functions.

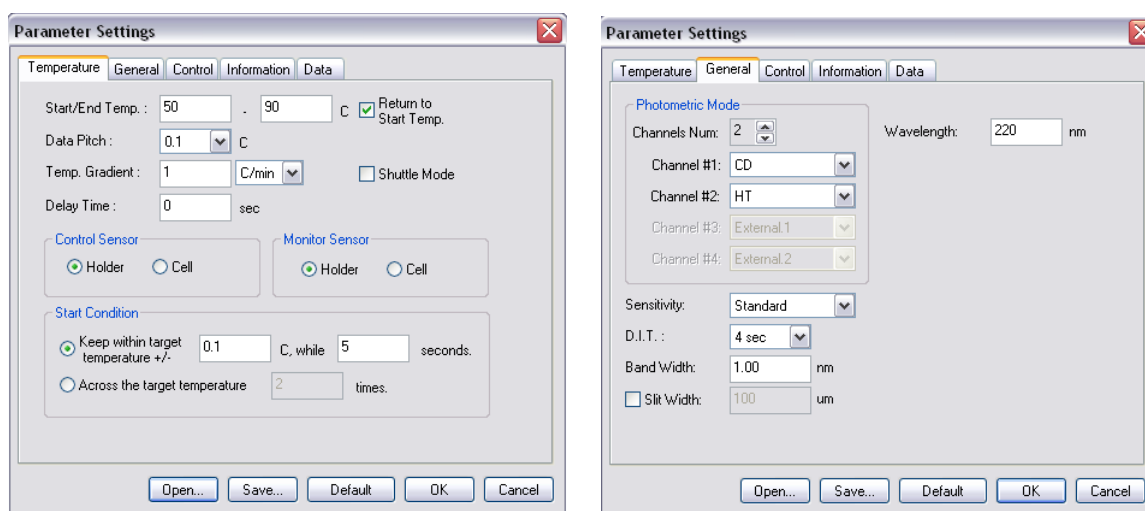


Figure 4.3 [Temperature] (left side) and [General] (right side) dialog boxes

- (2) Changing the parameters in the [Temperature] and the [General] dialog boxes  
Here, set them as shown in the following example (refer to Sections 3.1.1.1 and 3.1.1.2 for a description of and the limits for the following parameters).

[Temperature] menu

[Start/End Temp.]	50.0 – 90.0 °C
[Data Pitch]	0.1 °C
[Temp. Gradient]	1.0 °C/minute
[Delay Time]	0 second
[Return to Start Temp.]	ON
[Shuttle Mode]	OFF
[Control Sensor]	Holder
[Monitor Sensor]	Holder
[Start Condition]	Temp.: less than $\pm 0.1$ °C
	Delay time: 5 seconds

[General] menu

Channel #1	CD
Channel #2	HT

[Sensitivity]	Standard
[D.I.T.]	4 seconds
[Band Width]	1.0 nm
[Wavelength]	220 nm

**Note (1):** These parameters are merely given as an example and are not to be applied in every case.

**Note (2):** Refer to Sections 3.1.1.1 and 3.1.1.2 for more information regarding the following menus.

### [Temperature] menu

- 1) Set [Start/End Temp.].  
Enter the upper and the lower temperatures into the left and the right text boxes, respectively. To input the value in the [Start] box, for example, click its text box. A cursor appears in the text box, waiting for input. Delete unnecessary numerals and input the desired temperature using the numeric keys.
- 2) Set [Data Pitch].  
[Data Pitch] is a drop-down box. Clicking the arrow on the extreme right of the box displays a list of values.
- 3) Set [Temp. Gradient].  
[Temp. Gradient] is a drop-down box. Clicking the arrow on the extreme right displays a list of values.
- 4) Set [Delay Time].  
Enter the delay time (sec) into the text boxes. This time starts after the temperature has converged to the target temperature according to the target temperature criterion. To input a value for a parameter, click its text box. A cursor appears in the text box, waiting for input. Delete unnecessary numerals and input the desired value using the numeric keys.
- 5) Set [Return to Start Temp.]  
Insert a check mark in the [Return to Start Temp.] box if you want the temperature to return to the initial value (50°C, for example) after measurement has been completed.
- 6) Set [Shuttle Mode.]  
Insert a check mark in the [Shuttle Mode.] box if you want to use the shuttle drive (the temperature increases until the “End temp” is reached and then decreases to the “Start Temp.”).
- 7) Set [Control Sensor]  
Select the area for controlling the temperature. [Holder] and [Cell] control the temperature in the sample cell and inner cell, respectively.
- 8) Set [Monitor Sensor]  
Select the area for monitoring the temperature.
- 9) Set [Start Condition].  
Select either [Keep within target temperature +/-] or [Across the target temperature].  
CASE I: Enter the criterion value in the left side box and the waiting time in the right side box. This waiting time applies to the criterion, and is not the same as the [Delay time].

CASE II Enter the desired number in the [Across the target temperature] box. This is the number of times the actual temperature crosses the target temperature .

### [General] menu

1) Set [Photometric Mode]

Select the number of [Photometric Mode] by clicking the arrow on the extreme right. The menu of each channel is a drop-down box. Clicking the arrow on the extreme right displays a list of the contents.

2) 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.

3) Set [D.I.T.].

[D.I.T.] is a drop-down box. Clicking the arrow at the extreme right displays a list of D.I.T. values.

4) Sets [Band Width].

Input the half-width value in the [Band Width] text box.

5) Sets [Wavelength].

Input the desired wavelength into the [Wavelength] text box. To input [Wavelength] 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.

### [Control], [Information] and [Data] menus

Enter the appropriate settings in the [Control], [Information] and [Data] dialog boxes if necessary.

- (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 to Sections 3.1.1.1 and 3.1.1.4 regarding 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 following screen appears.

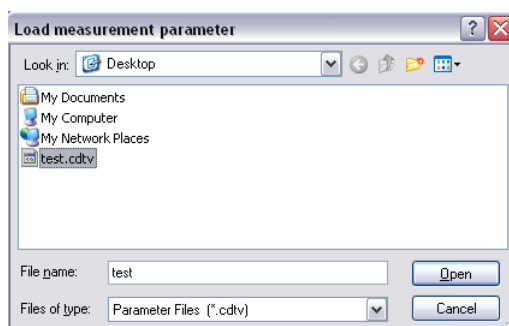


Figure 4.4 [Load measurement parameter] screen

Select a location to save the spectrum by clicking the arrow on the extreme right in the [Save in] box (in Figure. 4.4, "Desktop" is selected). Input a filename into the [Filename] text box. The extension (the letters appearing after ".") need not be entered. The output file is saved as a .cdtv format file. Clicking the <Save> button saves the parameters of the

[Variable Temperature Measurement] program on disk (the filename of Figure. 4.4 is “test”).

**Note:** The parameter file .cdtv contains both baseline and sample measurements when the [Baseline] menu is selected. It only contains sample measurement parameters when [Blank] or [None] is selected.

#### 4.2.4 Setting Sample and Measurement

(1) Setting sample

- 1) Prepare a cubic cell filled with phosphate buffer solution or Lyz solution, which is used for blank or sample measurement. Do not forget to put the top on the cell.
- 2) Insert the sample cell into the hole of the Peltier in an appropriate space.


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

**Note (2):** Ensure that the temperature of sample is correct. Refer to Section 4.2.2 for how to control the temperature of the sample and the sample cell holder.

**Note (3):** If the Peltier accessory is not registered in the [Temperature Interval Scan Measurement], [sample] - [Measure] menu is displayed in gray.

(2) Measurement

1) Baseline measurement

Selecting [Blank/Baseline] from the [Measure] menu (or clicking the button ) displays one of the following message dialog boxes.

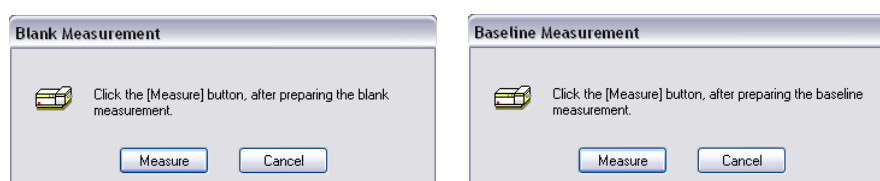





Figure 4.5 Message boxes for starting [Blank/Baseline] measurement

CASE I: The dialog depicted on the left side of Figure. 4.5 appears following the case using the parameters depicted in Section 4.2.3. (when the [Blank] menu was selected in the [Control] - [Parameters] dialog box). Clicking <Measure> starts the [Blank] measurement which is a one-point measurement. During measurement,  becomes inactive, as indicated by the gray icon  or selecting  - [Measure] from the [Variable Temperature Measurement] window (see Figure. 4.1) if you need to perform an emergency stop.

**Note:** In some cases performing the Blank measurement cannot remove distortion to the spectrum produced by the sample cell at high temperatures. This function should be employed after investigating the influence of strain at several temperatures.

CASE II: The dialog depicted on the right side of Figure. 4.5 appears when [Baseline] is selected, which is in the [Parameter] - [Measure] menu of [Variable Temperature Measurement] window (see Figure. 4.1). Clicking the <Measure> button starts the [Baseline] measurement and the following dialog appears.

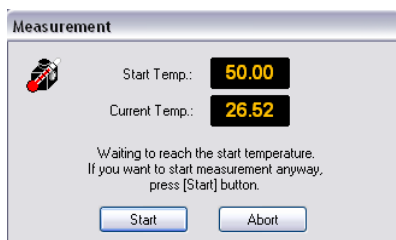


Figure 4.6 [Measurement] dialog box

During the measurement, the dialog box of Figure. 4.6 appears. Clicking the <Start> button and the data at [Current Temp.] is read. Clicking the <Abort> button interrupts the measurement immediately.

**Note (1):** The [Baseline] function is more effective than the [Blank] function for estimating relatively small CD values and its changes.

**Note (2):** When the <Abort> button is clicked the Measurement window displays the data acquired from the initial temperature up to the temperature reached when the measurement was interrupted. When interrupted, the acquired data cannot be used as for baseline correction.

Baseline data and its parameters can be read from .cdbtv format file. Select [Open Parameters...] in the [File] menu of [Variable Temperature Measurement] window. The following screen appears.

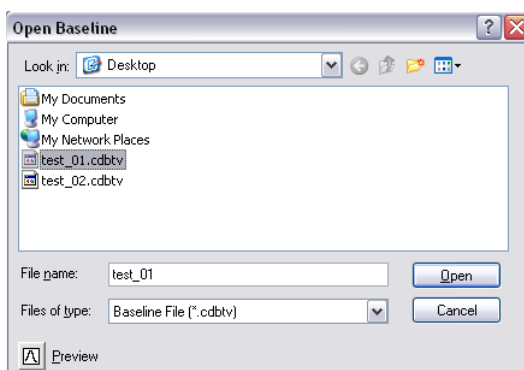


Figure 4.7 [Open Baseline] screen

Select the location to open the data from by clicking the arrow at the top of the [Open Baseline] box (in Figure. 4.7 “Desktop” is selected). Input a filename into the [Filename] text box. The extension (the letters that appear the letters appearing after “.”) need not be entered. Clicking the <Open> button loads the parameters into the [Variable Temperature Measurement] program from disk (the filename in Figure. 4.7 is “test\_01”).


**Note (1):** The data file .cdbtv contains data and parameters obtained in [Baseline] mode ([Blank] data cannot be opened and saved).

**Note (2):** When the [Open Baseline] menu is used, the [Baseline] menu must be selected, from the [Parameters...] - [Measure] menu of [Variable Temperature Measurement].

**Note (3):** After reading the data and parameters, the baseline parameters are updated in the [Variable Temperature Measurement] program. Confirm this by checking the text screen displayed at the right side of the [Variable Temperature Measurement] window (the current parameters for sample measurement are unchanged).

**Note (4):** If the parameters are changed in the [Parameters] - [Measure] menu, the existing data and parameters are not saved. This data should be saved or transferred to the [Spectra Analysis] program.

## 2) Sample measurement

Select [Sample] from the [Measure] menu (or click the  button) after performing procedure 1.

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

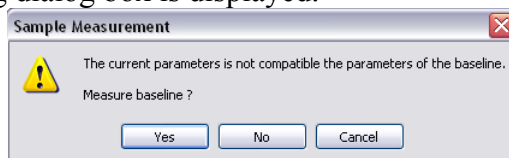



Figure 4.8 [Sample Measurement] message box

If the <Yes> button is clicked, the baseline measurement is carried out using the current parameters. If the <No> button is clicked, the sample measurement is carried out even if both parameters are different.

**Note (1):** The same measurement parameters should be employed for both the sample and baseline measurements.

**Note (2):** If these parameters are different, the corresponding menu displayed in the parameter box is displayed with red or yellow sign. If a red sign is displayed, no correction can be performed when there is no correction data. When a yellow sign is displayed, the correlation can be performed but its quality is will not be good.

Clicking the <Cancel> button interrupts the baseline measurement and the system waits for further instruction. To abort the measurement immediately, click the  button or select [Cancel] from the [Measure] menu. In this case, the following message box appears (this box does not appear in the case of baseline measurement).

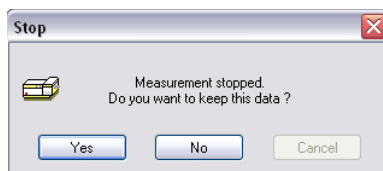


Figure 4.9 [Stop] message box

Measurement is interrupted immediately by clicking either the <Yes> or the <No> button.

CASE II: When [None] was selected from the [Parameters...] - [Measure] menu, the sample measurement is performed without baseline correction.

**Note (1):** When the <Abort> button is clicked the Measurement window displays the data acquired from the initial temperature up to the temperature reached when the measurement was interrupted. When the measurement is interrupted by clicking the <Yes> button, the acquired data can be used. When the <No > button is clicked, the acquired data cannot be used (it is just displayed on the screen).

**Note (2):** If parameters are changed in the [Parameters] - [Measure] menu, the existing data and parameters are not saved. The data should be saved or transferred to the [Spectra Analysis] program.


## 4.2.5 Saving Data and Parameters

This section describes how to save parameters, baseline data and sample data.

**Note:** Refer also to Section 3.1.1.5 for how to automatically save data.

### 4.2.5.1 Saving Parameters

Saves parameters onto disk.

(1) Select [Save Parameters...] from the [File] menu or click the  button which is in the [Variable Temperature Measurement] window. The following dialog box appears.

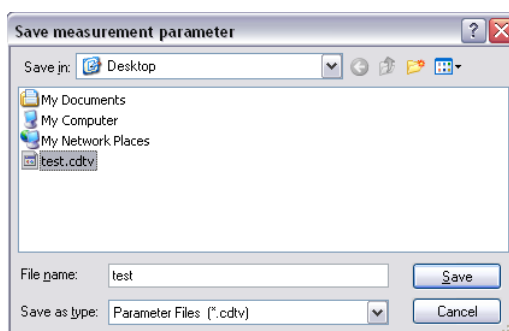


Figure 4.10 [Save measurement parameters] dialog box

- (2) Select a location to save the parameters by clicking the arrow on the top of the [Save in] box (in Figure. 4.10, "Desktop" is selected).
- (3) Input a filename in the [Filename] text box. The extension (the letters that appear the letters appearing after ".") need not be entered. The output file is saved as a .cdtv format

file.

- (4) Clicking the <Save> button saves the spectrum is on disk (in the example shown the filename is “test”).

**Note(1) :** The data file .cdtv contains both sample and blank measurement parameters when [Baseline] mode has been selected. When [Blank] or [None] mode is selected in the [Parameters...] - [Measure] menu , no blank parameters exist (Perform the [Blank] measurement again when [Blank] mode is selected)

**Note (2):** The parameters are specific for each accessory. If registering a different accessory, the current parameters are discarded and either the default parameters or the parameters registered by clicking the <OK> button in the [Parameters Setting] window are used.

#### 4.2.5.2 Saving Baseline Data

Saves a baseline spectrum to disk.

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

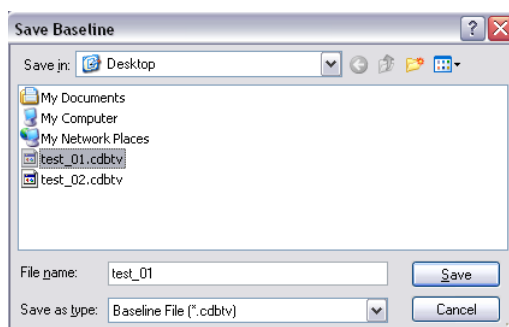


Figure 4.11 [Save Baseline] dialog box

**Note (1):** [Save Baseline...] is available only when the [Baseline] mode has been selected. ([Blank] data cannot be read or saved).

**Note (2):** The data file .cdbtv contains both baseline data and parameters.

- (2) Select a location to save the spectrum by clicking the arrow on the extreme right in the [Save in] box (in Figure. 4.11 “Desktop” is selected).
- (3) Input a filename into the [Filename] text box. The extension (the letters appearing the letters appearing after “.”) need not be entered. The output file is saved as a .cdbtv format file.
- (4) Clicking the <Save> button saves the spectrum to disk (the filename in the example is “test\_01”).

#### 4.2.5.3 Saving Sample Data

Saves an acquired sample spectrum to disk.

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



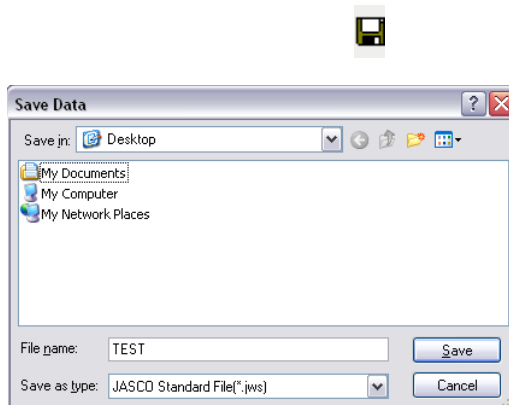


Figure 4.12 [Save Data] dialog box


**Note:** [Save Data...] is only available when sample measurement has finished.

- (2) Select a location to save the spectrum clicking the arrow at extreme right in the [Save in] box (in Figure. 4.12, “Desktop” is selected).
- (3) Input a filename in the [Filename] text box. The extension (the letters appearing 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 (in the example shown the filename is “TEST”).

**Note (1):** When the measurement is interrupted by clicking the <Yes> button, the acquired data can be saved as a .jws file. When the <No > button is clicked, the acquired data cannot be saved.

**Note (2):** Refer to Section 3.1.1.5 for how to use the auto saving data function.

#### 4.2.6 Sending Data to [Spectra Analysis]

Transfers an acquired spectrum to the [Spectra Analysis] window. Select [Analysis Send] from the [File] menu or click the button  the [Variable Temperature Measurement] window. The [Spectra Analysis] window is opened automatically.

**Note (1):** When the measurement is interrupted by clicking the <Yes> button, the acquired data is transferred to the [Spectra Analysis] program.

**Note (2):** Only the measurement parameters are sent to the [Spectra Analysis] program. If baseline parameter and baseline data are required, use [Save Parameters...] and [Save baseline], respectively.

**Note (3):** If [Interval Analysis] has already been started and the displayed data has not yet been saved, a message appears to that effect. Take appropriate action.

**Note (4):** Refer to Section 3.1.1.5 for how to use the auto data transfer function.

### 4.2.7 Printing Spectrum

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

<p><b>Note(1) :</b> Refer to “Spectra Analysis Manual” for more details.</p>
--

<p><b>Note (2):</b> Refer to Section 3.1.1.5 for how to use the auto printing data function.</p>
--

## 5. [Temperature Interval Scan Measurement] Menu Reference

Start the [Temperature Interval Scan Measurement] program. Open the following window by clicking the [Temperature Interval Scan Measurement] menu of [Spectra Manager].

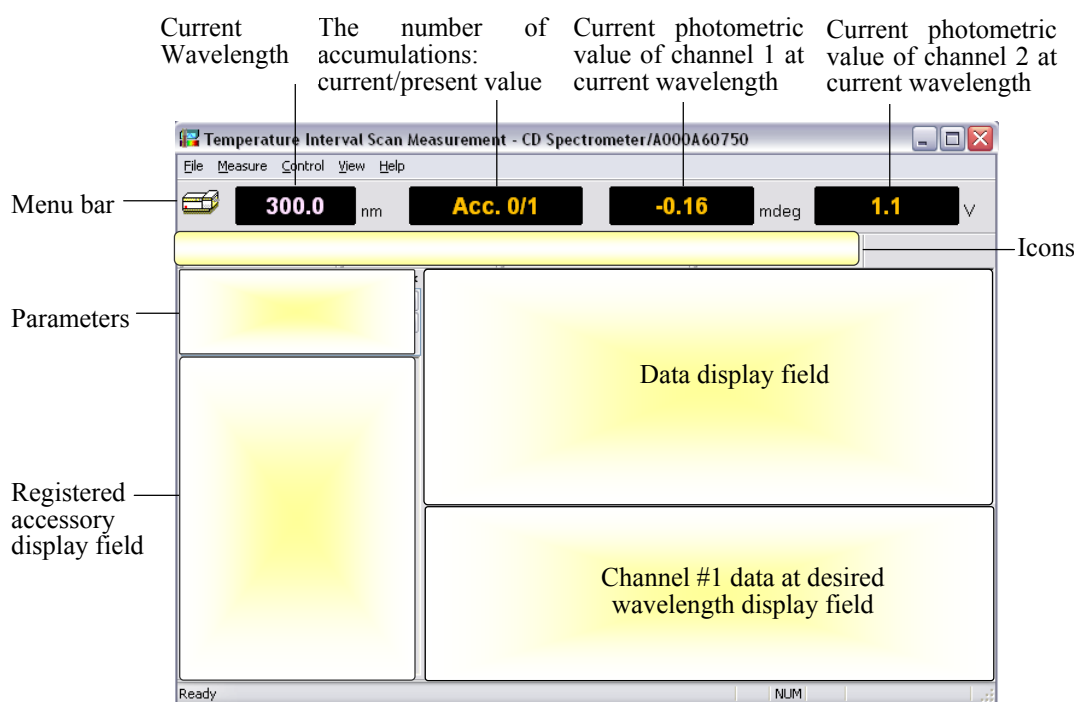


Figure 5.1 [Variable Temperature Measurement] window

**Note (1):** Figure. 1.1 shows one channel of data, but this program can display maximum four channels of data on Data display field simultaneously when measurement starts.

**Note (2):** Refer to Sections 2.2 and 2.3 regarding registration of the Peltier accessory.

**Note (3):** Refer to “J-800 Series Operation Manual” for how to start the [Spectra Manager] program

### [File] menu

- |                      |   |
|----------------------|---|
| [Save Data...]       | Saves the 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 Parameters...] | Opens variable temperature measurement parameters which are set in the [Parameter Settings] dialog box. The file format is .cdti. |
| [Save Parameters...] | Saves the measurement parameters as a .cdti format file.  |
| [Exit]               | Exits the [Spectra Measurement] window.   |

### [Measure] menu





- |                 |  |
|-----------------|--|
| [Parameters...] | Sets the measurement parameters, control area of Peltier (sample cell holder or sample cell), monitoring sensor area (sample cell holder or sample cell), toggles the auto-shutter control ON/OFF, edits |
|-----------------|--|

[Sample...]	comments and saves and loads measurement parameters and data.
[Cancel]	Starts measurement of sample.
	Stops blank and sample measurements.

### [Control] menu

[Move Wavelength...]	Moves the current wavelength to the desired value.
[CD Detector...]	Sets the detector (CD/ORD/LD/UV) sensitivity.
[Light Source...]	Toggles the light source ON/OFF. Displays/clears the light source operating time.
[Shutter...]	Opens or closes the shutter.
[Auto Zero]	Zeroes the photometric value of ORD-M (when installed).
[Select Accessory...]	Registers compatible accessories.
[PTC-423S]	Sets the temperature and the area controlling and monitoring the temperature (either the sample cell holder or the sample cell).

### [View] menu

[Select Graph...]	Selects the desired channel No. (default is channel 1).
[Overlay]	Overlays graphs.
[Scale...]	Sets the minimum and maximum values for the horizontal axis and/or the vertical axis.
[Pattern...]	Sets the color, style and width of lines (spectra).
[Font...]	Sets the font type for the axes values and/or unit(s).
[Grid...]	Displays or hides grid.
[Style...]	Sets the scale interval.
[Information Bar]	Displays or hides parameters such as those shown in Figure. 4.1.
[Toolbar...]	Displays or hides the toolbars shown in Figure. 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 Figure. 5.1.
[Temp. Monitor Bar]	Displays holder temp., cell temp., ideal temp. and/or given temp. at each measurement point.
[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 the measurement parameters, control areas of Peltier (sample cell holder or sample cell), monitoring sensor portion (either the sample cell holder or the sample cell), turns auto-shutter control ON/OFF, edits comments and saves and loads measurement parameters and data. The parameters dialog box is made up of five dialog boxes: [Temperature], [General], [Control], [Information] and [Data]. They can be changed by clicking the appropriate tab at the top of the box.

#### 5.1.1.1 [Temperature] Dialog Box

Sets the measurement parameters for the temperature.

**Note:** The menus of the [Temperature] dialog box depicted in Figure.5.2 are the same as those of [Variable Temperature Measurement].

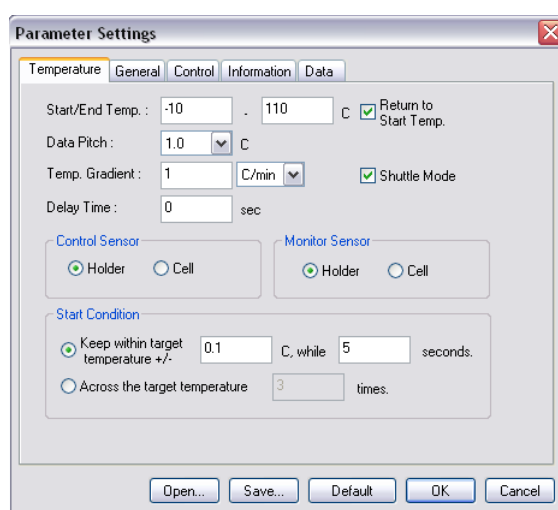


Figure 5.2 [Temperature] dialog box

#### Menu

- |                   |  |
|-------------------|--|
| [Start/End Temp]  | Sets the initial temperature (box on the left) and final temperature (box on the right) temperatures and wavelength (long wavelength end). The temperature increase as measurement is performed. The temperature range is -10.0 – 110.0°C and the temperature can be specified to the first decimal place. |
| [Data Pitch]      | Selects the data acquisition interval by clicking the arrow on the extreme right of the [Data Pitch] box. Range: 0.1 – 10.0°C.   |
| [Temp. Gradient]  | Sets the rate of temperature increase and decrease (temp./time). The units °C/minute or °C/hour can be selected by clicking the arrow on the extreme right of the box. Range: 0 – 10 °C/min and 0 – 600 °C/hr. It can be specified to the sixth decimal place.   |
| [Delay Time]      | Sets the delay time, which is the time before the measurement commences after the target temperature has been reached. Range: 0 sec – 3600 sec, where only integers can be entered.  |
| [Return to Start] | Returns to the [Start] temperature when measurement has finished.  |

Temp]	Put a check mark in the box if needed.
[Shuttle mode]	Performs measurement by decreasing the temperature after finishing the usual increasing temperature measurement. Put a check mark in the box if needed.
[Control Sensor]	Selects the area, in the sample cell [Holder] or the inner cell [Cell] for controlling the temperature. Select either [Holder] or [Cell] by clicking one of these options.
[Monitor Sensor]	Selects the area, in the sample cell [Holder] or the inner cell [Cell] for monitoring the temperature. Select either [Holder] or [Cell] desired by clicking one of these options.
[Start Condition]	Two types of criteria for attaining the target temperature are offered. CASE I: Determines the temperature range (°C) and the time (seconds) after the temperature enters the specified temperature range. The ranges are 0 – 10°C and 0 – 60 sec, respectively. They can be specified to the first decimal place and as an integer, respectively. CASE II: Determines the number of crossing points (times) with the target temperature. Range: 0 – 10 times.

### 5.1.1.2 [General] Dialog Box

Sets other measurement parameters besides the temperature.

**Note:** Menus in the [General] dialog box depicted in Figure. 5.3 are the same as those in [Spectra Measurement] except for [Cycle Times] and [Cycle Interval].

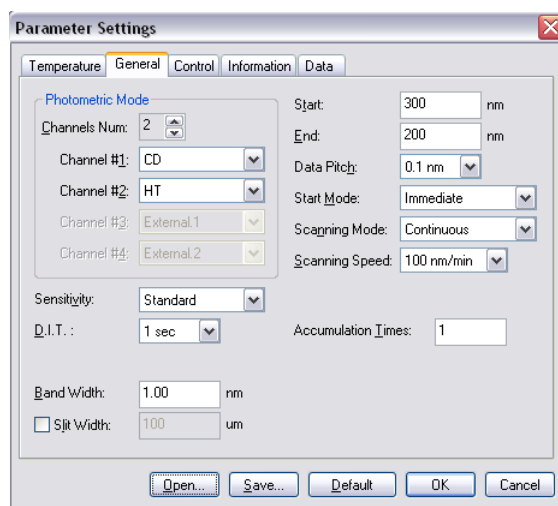


Figure 5.3 [General] dialog box

### Menu

[Channel Num]	Maximum of four channels. Four data types can be acquired simultaneously.
[Channel #1]	The selectable range varies with the optional accessory being used. CD: Circular dichroism signal, which is measured with ~AC/DC at 50 kHz. CD/DC: This is the same as for 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 used for testing the spectrometer.

LD (when the LD accessory is installed): Linear dichroism signal, which is measured with ~AC/DC at 100 kHz.

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

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

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

FDCD/DC (when the 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).						
[Sensitivity]	Selects the sensitivity from the following drop-down list. <table><tr><td>Low</td><td>Up to 1000 mdeg</td></tr><tr><td>Standard</td><td>Up to 200 mdeg</td></tr><tr><td>High</td><td>Up to 5 mdeg</td></tr></table>	Low	Up to 1000 mdeg	Standard	Up to 200 mdeg	High	Up to 5 mdeg
Low	Up to 1000 mdeg						
Standard	Up to 200 mdeg						
High	Up to 5 mdeg						
[D.I.T.]	Digital integration time per data point. 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. It 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 a drop-down list. Effective value extends to msec 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 triggered 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 varied.
- [Scanning Speed]     Selects a wavelength scanning speed. Can be entered when the scan mode is set to [Continuous].
- [Accumulation]     Sets the number of the accumulations for a measurement. Can be entered by inserting a check mark. Range: 1 – 999 times.

**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 the [D.I.T.] or [Data Pitch.] or [Scanning Speed] dialogs, an error message will be displayed.

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

**Note (3):** The acceptable ranges of values for the [Band Width] and [Wavelength] are not the same as those for the instrument. Refer to the “J-815 Hardware Manual” for their specification.

**Note (4):** 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.



### 5.1.1.3 [Control] Dialog Box

Toggles auto shutter driving ON/OFF.

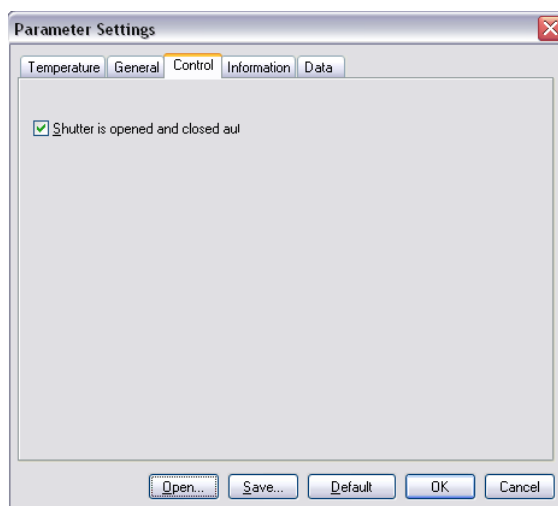


Figure 5.4 [Control] dialog box

### Menu

#### [Auto shutter]

Automatically opens the shutter just before measurement starts and closes it at the end of the measurement. Put a check mark if this function is necessary.

### 5.1.1.4 [Information] Dialog Box

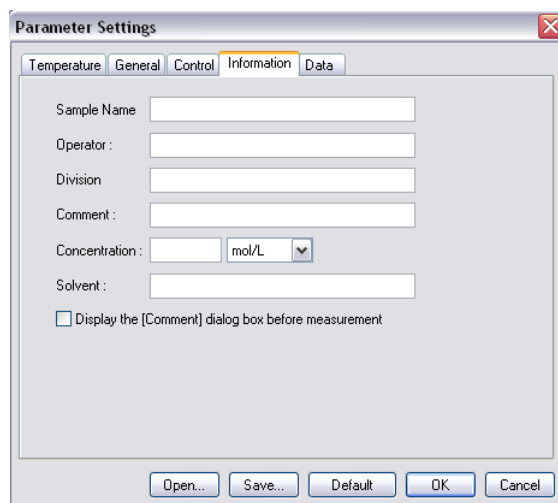


Figure 5.5 [Information] dialog box

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 following concentration units can be selected: mol/l, mmol/l,  $\mu$ mol/l, nmol/l, w/v%, ppm and ppb.

### 5.1.1.5 [Data] Dialog Box

Sets automatic saving, transfers data to Spectra Analysis and prints out spectra.

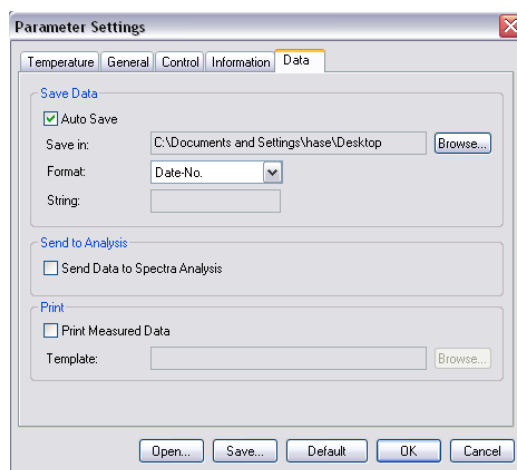


Figure 5.6 [Data] dialog box

[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 a directory where files are to be saved in the dialog box. This is useful for repeated measurements.

[Save in]

Enter the file and directory name. The <Browse...> button is useful for selecting the directory 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...
String-No.	Displays the filename given in the [String] box and the 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]

Allows you to define your preferred filename, which is displayed as "String-No".

[Print]

Sets 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 a directory where files are to be saved in the dialog box. This is useful for repeated measurements.

[Send data to Spectra Analysis]

Automatically transfers data to the [Spectra Analysis] program.

**Note (1):** Page setup for printing out must be set in the [JASCO Canvas] window.

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

### 5.1.1.6 Common function

The following buttons can be used in all screens, [Temperature], [General], [Control], [Information] and [Data].

- |           |  |
|-----------|--|
| <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 disk.<br>Clicking this button displays the [Open] dialog box. Selecting a baseline data file and clicking the <Open> button loads the baseline data into memory. The baseline data is found in .cdti format files. |
| <Save>    | Saves the parameters in a .cdti format file.   |
| <Default> | Reverts to the default parameters.   |

### 5.1.2 [Monitor Parameters...]

Displays the photometric value of channel #1 at the desired wavelength. Four different wavelengths can be selected in the wavelength range between the [Start] and [End] wavelengths which are specified in [General] - [Parameters...] in the [Temperature Interval Scan Measurement] window.

- (1) Select [Monitor Parameters...] - [Measure] in the [Temperature Interval Scan Measurement] window. The window of Figure 5.7 appears.

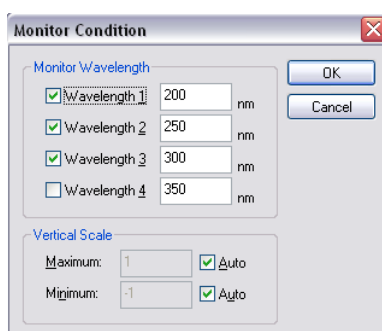


Figure 5.7 [Monitor Condition] dialog box

**Note:** Ensure the power supplies of the spectrometer and the Peltier accessory are turned ON, the COM ports are set appropriately and the accessory is registered in [Administrative Tools]. Refer also to Section 2.2 for more information.

- (2) Insert a check mark in [Wavelength #] of [Monitor Wavelength] and enter the desired wavelength into the right side box. For example, if the wavelength region was set from 200 nm to 300 nm in [Parameters...], there are three available photometric modes, namely 200 nm, 250 nm and 300 nm (350 nm is not displayed).
- (3) The vertical scale can be adjusted automatically or manually. The former is achieved by inserting a check mark into [Minimum] and/or [Maximum]. The latter is by entering the desired value(s) into the [Minimum] and/or [Maximum] boxes.

## 5.2 [Control] Menu

### 5.2.1 [Select Accessory...]

Refer to Section 2.3 for details. [PTC-423S] are displayed in the [Control] menu after registering the Peltier accessory. Selecting [PTC-423S] will result in the following dialog box being displayed.

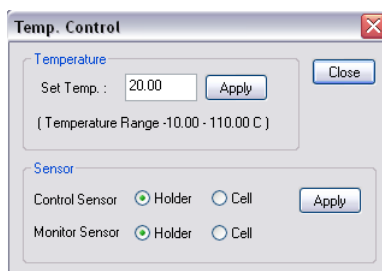


Figure 5.8 [Temp. Control] dialog box

[Set Temp.]	Sets temperature. Range: -10 nm to 110 nm.
<Apply>	Applies the set temperature.
[Control Sensor]	Area controlling temperature. <Holder>: sample cell holder, <Cell>: sample cell.
[Monitor Sensor]	Area monitoring temperature.
<Apply>	Applies the area.
<Close>	Closes the dialog box of Figure. 5.8.

**Note:** The Peltier accessory should be registered whenever the temperature controller is used. Otherwise, the temperature cannot be controlled.

### 5.2.2 [Move Wavelength...]

Moves the wavelength to the desired value.

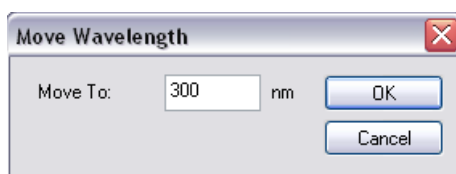


Figure 5.9 [Move Wavelength] dialog box

[Wavelength]	Text box for input. Range: 165 nm to 1100 nm.
<OK>	Moves the wavelength to the set wavelength.
<Cancel>	Closes the dialog box without changing the previous wavelength setting.

### 5.2.3 [CD Detector...]

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

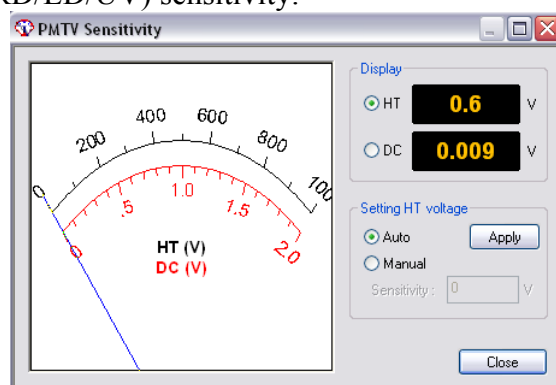


Figure 5.10 [PMTV Sensitivity] dialog box

- [Display] Changes the meter indication (displayed on the right side of Figure. 5.10) 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 the option button. If [Manual] is selected, input [Sensitivity] and click the <Apply> button. Set range: 0 to 1000 V
- <Close> Transfers the set value to the spectrometer and closes the dialog box.

**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 DC. If it is not DC, the data is not displayed in the [Spectra Measurement] window and it cannot be acquired.

### 5.2.4 [Light Source...]

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



Figure 5.11 [Light Source Control] dialog box

- [Xe Lamp] Turns the lamp ON/OFF. The icon is toggled by clicking it.
-  Icon indicating light is turned on.
-  Icon indicating light is turned off.

The operating time of the lamp is displayed in Figure. 5.11. (0.0 hour in this case)

- <OK> Turns the lamp ON/OFF.
- <Cancel> Closes the dialog box without changing anything.

**Note:** If the light source does not come on, try to turn it on several times. If you still have problems, contact your local JASCO distributor.

### 5.2.5 [Shutter...]

Opens or closes the shutter. Only effective for an instrument having a shutter.

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

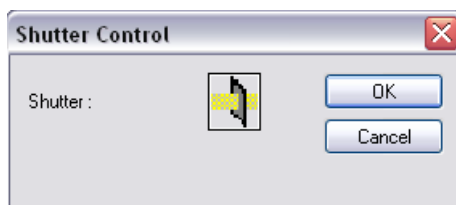


Figure 5.12 [Shutter Control] dialog box

[Shutter] Turns the shutter ON/OFF. The icon is toggled by clicking it.



Icon indicating that shutter is open.

Icon indicating that shutter is closed.

<OK> The shutter opens or closes.

<Cancel> Closes the dialog box without changing anything.

**Note (1):** Closing the shutters zeroes the HT voltage. Confirm this in the [CD Detector...] dialog box (Figure. 5.10) if necessary.

**Note (2):** When the spectrometer is turned ON, the shutter automatically opens. Check the front LED to see if the shutter is ON/OFF in this case.

### 5.2.6 [ORD-M Zero Clear]

This is effective only when ORD-M is installed.

## 6. Introduction to [Temperature Interval Measurement] Program

This section contains the procedures for starting up the [Variable Temperature Measurement] program, measuring sample, saving the measured data on disk and printing out the result to familiarize the operator with operation.

**Note (1):** Refer to the instruction manuals for accessories for how to start the spectropolarimeter and accessories and to register the accessories. Here, the description starts from the startup of [Variable Temperature Measurement] program from the [Spectra Manager] program.

**Note (2):** Here, it is assumed that the Peltier-type single cell holder has been connected.

### 6.1 Operation Overview

Starting spectrometer	Refer to "Hardware manual".
↓	
Sample preparation	See "6.2.1".
↓	
Starting Temperature Variable Measurement Program	See "6.2.2".
↓	
Registering Accessories on [Variable Temperature Measurement]	See to "2.3".
Setting Parameters	See "6.2.3".
↓	
Setting Sample and Measurement	See "6.2.4".
↓	
Saving Data and Parameters	See "6.2.5".
↓	
Sending Data to [Spectra Analysis]	See "6.2.6".
↓	
Printing Spectrum	See "6.2.7".

## 6.2 Measuring, Saving and Printing Data

How to measure, save and print data using 0.0074 mol/l Lysozyme (Lyz) in water solution with 10 mM phosphate buffer is explained. (This is the same as the example used for [Variable Temperature Measurement] program.)

### 6.2.1 Sample Preparation

Prepare about 1 mg Lyz and put it into 10 ml of 10 mM phosphate buffer solvent. Put the prepared sample into a 0.1 cm cell.

**Note (1):** The Lyz solution should be prepared immediately prior to performing the measurement.

### 6.2.2 Starting the Temperature Variable Measurement Program

**Note:** Ensure the power supplies of the spectrometer and the Peltier accessory are turned ON, the COM ports are set appropriately and the accessory is registered in [Administrative Tools]. Refer also to Section 2.2 for more information.

- (1) Double-click the [Temperature Variable Measurement] menu in the [Spectra Manager] window. The window shown in Figure. 1.1 appears.
- (2) Register the Peltier accessory following the procedure described in Section 2.3. The [Temperature Variable Measurement] window appears as shown below.

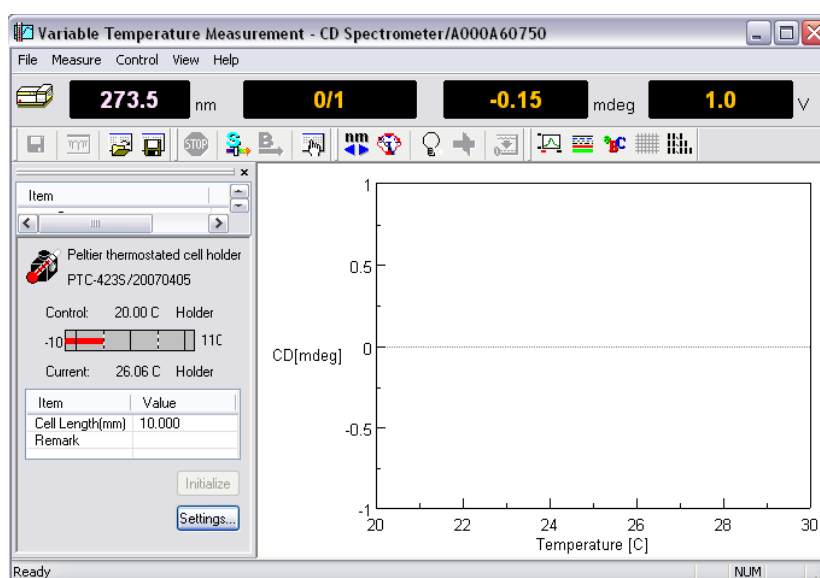


Figure 6.1 [Temperature Variable Measurement] window



- (3) Select [PTC-423S] from the [Control] menu or click <Settings...> button of Figure. 6.1. The following dialog box appears.

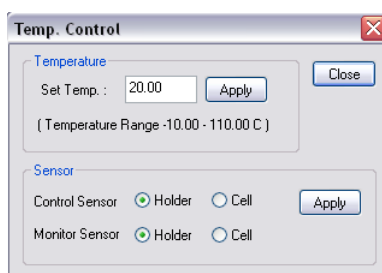



Figure 6.2 [Temp. Control] dialog box

- (4) Enter the desired temperature into the text boxes and click the <Apply> button. To input a value for a parameter click its text box. A cursor appears in the text box, waiting for input. Delete unnecessary numerals and input the desired value using the numeric keys.
- (5) Set desired menus for [Control Sensor] and [Monitor Sensor], which are the areas for controlling temperature and monitoring the temperature, respectively.
- (6) Clicking the <Close> button registers the temperature.

**Note (1):** After clicking the < Close> button, the “Stop” sign in the front panel of Peltier accessory becomes a “Start” sign.

**Note (2):** Refer to the “PTC-423 Manual” for how to use the accessory safely and correctly.

### 6.2.3 Setting Parameters

- (1) Click the  on or select [Parameters...] from the [Measure] menu of Figure. 6.1. The following dialog box appears. The parameters setting dialog box is composed of the [Temperature], [General], [Control], [Information] and [Data] dialog boxes. Clicking a tab at the top of the dialog box changes the dialog box. Refer to Section 3.1.1 for descriptions of these functions.

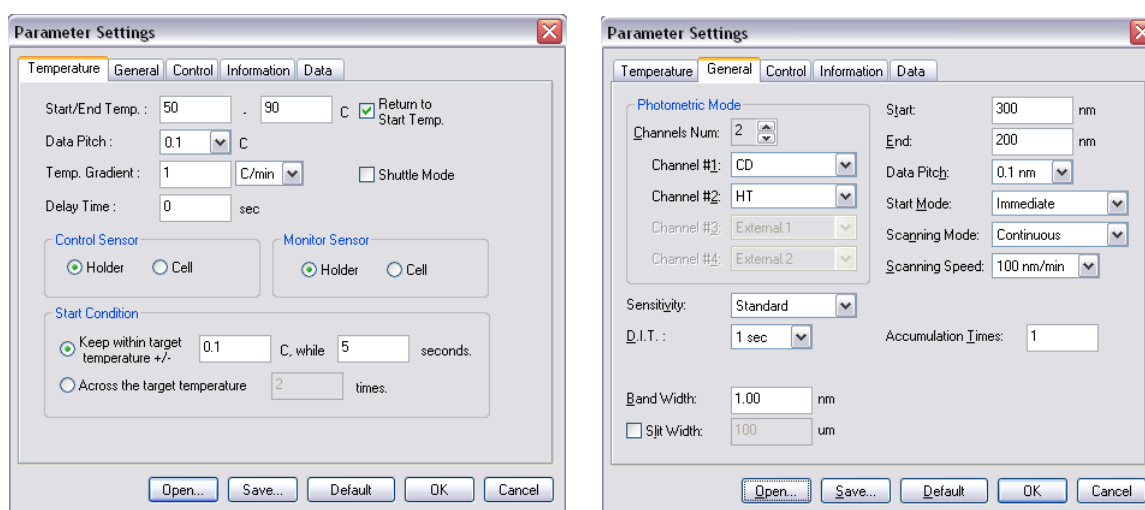


Figure 6.3 [Temperature] (left side) and [General] (right side) dialog boxes

- (2) Changing the parameters in the [Temperature] and the [General] dialog boxes  
Here, set them as shown in the following example (refer to Section 3.1.1.1 and 3.1.1.2 for a description of and the limits for the following parameters).

[Temperature] menu

[Start/End Temp.]	50.0 – 90.0 °C
[Data Pitch]	0.1 °C
[Temp. Gradient]	1.0 °C/minute
[Delay Time]	0 second
[Return to Start Temp.]	ON
[Shuttle Mode]	OFF
[Control Sensor]	Holder
[Monitor Sensor]	Holder
[Start Condition]	Temp.: less than $\pm 0.1^{\circ}\text{C}$
	Delay time: 5 seconds

[General] menu

Channel #1	CD
Channel #2	HT
[Sensitivity]	Standard
[D.I.T.]	4 seconds
[Band Width]	1.0 nm
[Wavelength]	220 nm

**Note (1):** These parameters are merely given as an example and are not to be applied in every case.

**Note (2):** Refer to the Appendix of the “J-815 Hardware Manual” for setting appropriate values for the [Scanning Speed] and the relationship between [D.I.T.], the S/N ratio and [Accumulation Times].

**Note (3):** Refer to Sections 5.1.1 and 5.1.2 for more information regarding the following menus.

**[Temperature] menu**

- 1) Set [Start/End Temp.].  
Enter the upper and the lower temperatures into the left and right text boxes, respectively. To input the value in the [Start] box, for example, click its text box. A cursor appears in the text box, waiting for input. Delete unnecessary numerals and input the desired temperature using the numeric keys.
- 2) Set [Data Pitch].  
[Data Pitch] is a drop-down box. Clicking the arrow on the extreme right of the box displays a list of values.
- 3) Set [Temp. Gradient].  
[Temp. Gradient] is a drop-down box. Clicking the arrow on the extreme right displays a list of values.
- 4) Set [Delay Time].  
Enter the delay time (sec) into the text boxes. This times starts after the temperature has

converged to the target temperature according to the target temperature criterion. To input a value for a parameter, click its text box. A cursor appears in the text box, waiting for input. Delete unnecessary numerals and input the desired value using the numeric keys.

- 5) Set [Return to Start Temp.]  
Insert a check mark in the [Return to Start Temp.] box if you want the temperature to return to the initial one (50°C, for example) after measurement has been completed.
- 6) Set [Shuttle Mode.]  
Insert a check mark in the [Shuttle Mode.] box if you want to use the shuttle drive. (the temperature increases until the “End temp” is reached and then decreases to the “Start Temp.”).
- 7) Set [Control Sensor]  
Select the area for controlling the temperature. [Holder] and [Cell] control the temperature in the sample cell and inner cell, respectively.
- 8) Set [Monitor Sensor]  
Select the area for monitoring the temperature.
- 9) Set [Start Condition].  
Select either [Keep within target temperature +/-] or [Across the target temperature].  
CASE I: Enter the criterion value in the left side box and the waiting time in the right side box. This waiting time applies to the criterion, and is not the same as the [Delay time].  
CASE II Enter the desired number in the [Across the target temperature] box. This is the number of times the actual temperature crosses the target temperature .


#### **[General] menu**

- 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 an external trigger is not required, such is the case when using stopped flow accessories, select 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. For example, to input the value in [Start] click its text box. A cursor appears in the text box, waiting for input. Delete unnecessary numerals and input the desired 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, for example gas phase CD measurements, 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 [D.I.T.] values. This is restricted by the [Scanning Speed] and by the [Band Width]. For example, suppose that the [Scanning Speed] and the [Band Width] have the values given in Figure. 4.2. 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 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.

### [Control], [Information] and [Data] menus

Enter the appropriate settings in the [Control], [Information] and [Data] dialog boxes if necessary.

- (1) 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 to Sections 3.1.1.1 and 3.1.1.4 regarding usage of <Open...>, <Save...>, <Default> and <Cancel>.
- (2) 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 following screen appears. 

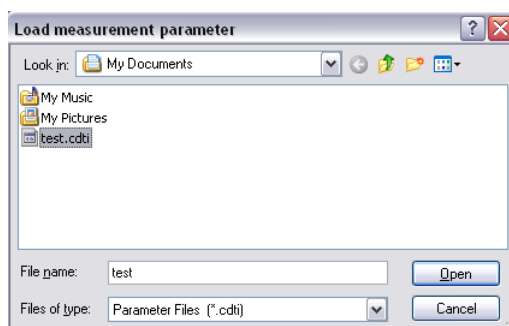


Figure 6.4 [Load measurement parameter] screen

Select a location to save the spectrum by clicking the arrow on the extreme right in the [Save in] box (in Figure. 6.4, “My Documents” is selected). Input a filename into the [Filename] text box. The extension (the letters appearing after “.”) need not be entered. The output file is saved as a .cdti format file. Clicking the <Save> button saves the parameters of the [Variable Temperature Measurement] program on disk (the filename of Figure. 6.4 is “test”).

**Note:** The parameter file .cdti has contains only [sample] data since the [Temperature Interval Scan Measurement] program does not support for [Blank] measurement.

### 6.2.4 Setting Sample and Measurement


- (1) Setting sample
  - 1) Prepare a cubic cell filled with phosphate buffer solution or Lyz solution, which is used for blank or sample measurement. Do not forget to put the top on the cell.
  - 2) Insert the sample cell to the hole of Peltier in an appropriate space.
  - 3) Ensure that the power of Peltier accessory is turned ON and the temperature description of Figure. 2.13 is displayed as shown in Figure. 6.1.

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

**Note (2):** Ensure the temperature of sample. Refer to Section 4.2.2 for how to control the temperature of the sample and the sample cell holder.

**Note (3):** If Peltier accessory is not registered in the [Temperature Interval Scan Measurement], [sample] - [Measure] menu is displayed in gray.

## (2) Measurement

Select [Sample] from the [Measure] menu (or click the  button). The measurement program then runs and displays the following dialog box.

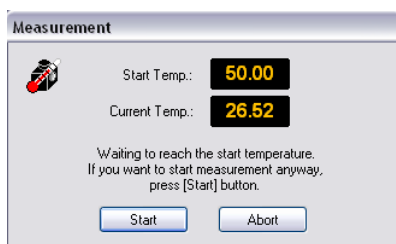




Figure 6.5 [Measurement] dialog box

Clicking the <Measure> button of Figure. 6.4 acquires data at 26.5°C and starts the [Spectra Measurement] program following the setting of Figure. 6.3. During measurement, becomes inactive, as indicated by the gray icon . Click <Abort> when Figure. 6.4 is displayed and the measurement stops immediately. When the [Spectra Measurement] program is running, click  or select [Cancel] - [Measure] from the [Temperature Interval Measurement] window. In both cases, the following dialog box appears.

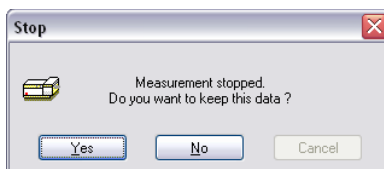


Figure 6.6 [Stop] dialog box

- <Yes> : [Temperature Interval Measurement] program is interrupted. The data is displayed and saved until the measurement was interrupted.
- <No.> : [Temperature Interval Measurement] program is interrupted. The data is displayed until the measurement was interrupted. But the data is not saved.
- <Cancel> : Continues running the [Temperature Interval Measurement] program.

**Note (1):** When the <Abort> button is clicked the Measurement window displays the data acquired from the initial temperature up to the temperature reached when the measurement was interrupted. When the measurement is interrupted by clicking the <Yes> button, the acquired data can be used. When the <No > button is clicked, the acquired data cannot be used (it is just displayed on the screen).

**Note (2):** If parameters are changed in the [Parameters] - [Measure] menu, the existing data and parameters are not saved. The data should be saved or sent to the [Spectra Analysis] program.

**Note (3):** A blank measurement can be carried out in the same way from the [Sample] - [Measure] menu. The subtraction between the sample and blank data should be carried out in the [Spectra Analysis] program.


## 6.2.5 Saving Data and Parameters

This section describes how to save parameters and sample data.

**Note:** Refer also to Section 3.1.1.5 for how automatically save data.

### 6.2.5.1 Saving Parameters

Saves parameters onto disk.

- (1) Select [Save Parameters...] from the [File] menu or clicking the  button, which is in the [Temperature Interval Measurement] window. The following dialog box appears.

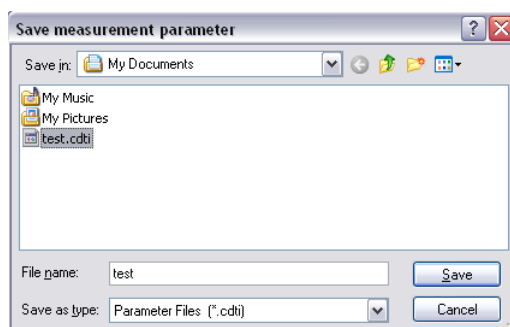


Figure 6.7 [Save measurement parameter] dialog box


- (2) Select a location to save the parameters by clicking the arrow on the top of the [Save in] box (in Figure. 6.7, “Desktop” is selected).
- (3) Input a filename in the [Filename] text box. The extension (the letters appearing after “.”) need not be entered. The output file is saved as a .cdti format file.
- (4) Clicking the <Save> button saves the spectrum is on disk (in the example the filename is “test”)

**Note(1) :** The parameter file .cdti has contains only [sample] data since [Temperature Interval Scan Measurement] does not support for [Blank] measurement.

**Note (2):** The parameters are specific for each accessory. If registering a different accessory, the current parameters are discarded and either the default parameters or the parameters registered by clicking the <OK> button in the [Parameters Setting] window are used.

### 6.2.5.2 Saving Sample Data

Saves a measured sample spectrum to disk.

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

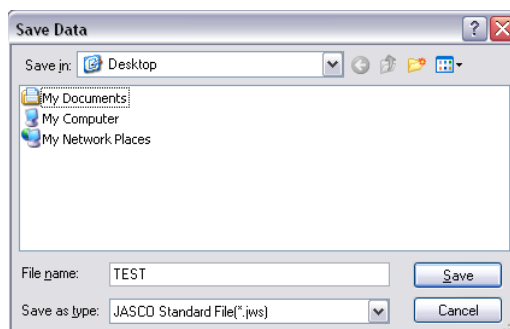


Figure 6.8 [Save Data] dialog box


**Note:** [Save Data...] is only available when sample measurement is finished.

- (2) Select a location to save the spectrum by clicking the arrow on the extreme right in the [Save in] box (in Figure. 6.8 “Desktop” is selected).
- (3) Input a filename in the [Filename] text box. The extension (the letters appearing after “.”) need not be entered. The output file is saved as a .jws format file.
- (4) Clicking the <OK> button saves the spectrum onto disk (the filename in the example is “TEST”).

**Note (1):** When the measurement is interrupted by clicking < Yes> button, the acquired data can be saved as a .jws file. When the <No > button is clicked, the acquired data cannot be saved.

**Note (2):** Refer to Section 3.1.1.5 for how to use the auto saving data function.

### 6.2.6 Sending Data to [Spectra Analysis]

Transfers an acquired spectrum to the [Spectra Analysis] window. Select [Analysis Send] from the [File] menu or click the  button in the [Variable Temperature Measurement] window. The [Spectra Analysis] window is opened automatically.

**Note (1):** When the measurement is interrupted by clicking the < Yes> button, the acquired data is transferred to the [Spectra Analysis] program.

**Note (2):** The only measurement parameters are sent to the [Spectra Analysis] program. If baseline parameter and baseline data are required, use [Save Parameters...] and [Save baseline], respectively.

**Note (3):** If [Interval Analysis] has already been started and the displayed data has not yet been saved, a message appears to that effect. Take appropriate action.

**Note (4):** Refer to Section 3.1.1.5 for how to use the auto data transfer function.



### 6.2.7 Printing Spectrum

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

<p><b>Note(1) :</b> Refer to “Spectra Analysis Manual” for more details.</p>
--

<p><b>Note (2):</b> Refer to Section 3.1.1.5 for how to use the auto printing data function.</p>
--

JASCO Corporation  
2967-5, Ishikawa-machi, Hachioji  
TOKYO, JAPAN

Printed in Japan