CONTROL DEVELOPMENT, Inc.

Price Performance Leader In Spectroscopy and Optical Components

Spectrometer Application Software Manual

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Before You Begin

Warning and Caution

WARNING

Disconnect your computer's power supply from its AC power source before you install or remove the spectrometer cards from your PC. Failure to do this can result in equipment damage. Some circuitry on the PC can continue to operate even though the front panel power switch is off.

CAUTION

Electrostatic discharge can damage your spectrometer card. Avoid touching the edge of the spectrometer card, and always handle the spectrometer by holding the case, **Figure 1.**

Your spectrometer was built with dedicate electronic and optical components. It was precisely calibrated to optimize its performance. Handle your spectrometer with great care to keep your spectrometer trouble-free and other problems in the future.

- Do not shake or bump the spectrometer against any hard objects that may cause damage to the electrical components and / or misalignment of the optics inside the spectrometer.
- Always replace the end plastic cap on the fiber optic cable connector to keep it clean and free of dust when not using the spectrometer. See **Figure 2.**
- Do not bump the fiber optic cable connector of the spectrometer against any hard objects as it can damage the connector and consequently damage the fiber optic cable that connects directly to the inside optic assembly. See **Figure 2.**

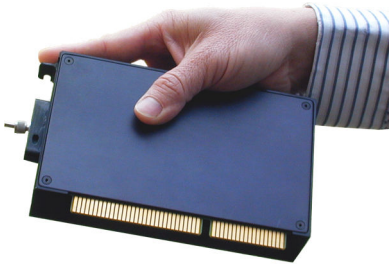


Figure 1: Properly handling the spectrometer by its case

Figure 2: Fiber cable connector with end cap on.

SHIPPING CAUTION

If a spectrometer needs to be shipped to a different location, please follow the instructions below to protect the spectrometer from damage and wear.

1. Make sure to use a non-collapsible cardboard box with plenty of peanut and bubble wrap around the spectrometer.
2. Keep the spectrometer in the center of the shipping package to prevent it from moving.
3. Protect the fiber optic cable connector, **Figure 2.** This fiber optic cable connector can easily be damaged during shipment. Follow the instructions below to protect it.

    a. First, cut a strip of cardboard (**A**) roughly 6" long and 2" wide. **Figure 3.** Fold the strip of cardboard a couple times so it would make a small loop (**B**). Apply a piece of tape to the crease so it won't come unfolded.

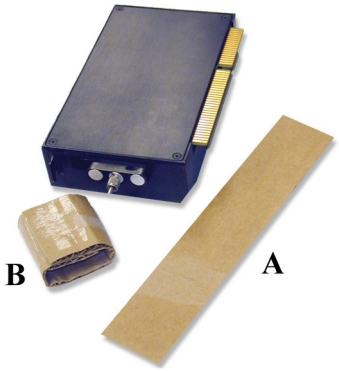


Figure 3: A strip of cardboard (A), was folded to make a small loop (B)

    b. Insert the folded cardboard (**B**) over the fiber cable connector on the spectrometer to protect it during shipment. **Figure 4.**

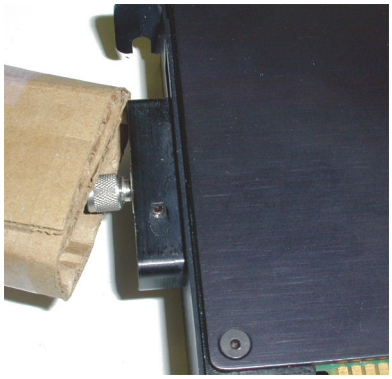
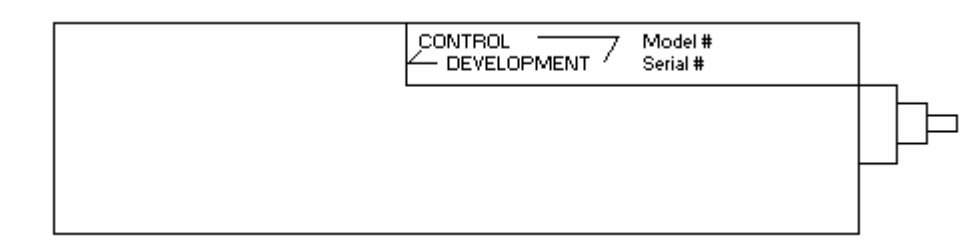


Figure 4: Placing the folded cardboard (B) over the fiber optic cable connector.

Chapter 1
Installation and Setup

1. Unit Identification

CDI manufactures and supports several different types of spectrometers. To help you identify your unit, a label is located on the top of the unit. The following chart should help you make a positive Identification.



Model # card-type-resolution-spectral response-1 stage cooler:-10º-interface type/dispersion/slit size

The model number will give the name of the card, the type of spectrometer, the spectral range in nanometers, 1 or 2 stage cooler in Celsius temperature, the interface type, dispersion, and the slit size used in the construction of the unit. There are four basic units available:

Type	**Description**
MPP	Multi-Pin Phased
PDA	Photo Diode Array
NIR	Near Infrared
RAMAN	Raman

The serial number is a unique identification number that CDI tech support will request in response to issues with a spectrometer, including RMA submissions.

PDA and NIR Plug-in Card
ISA Interface

PDA, NIR, MPP and RAMAN
USB Interface

NIR Plug-in Card
ISA Interface

Portable PDA and NIR

USB (1.0/1.1/2.0) Standalone Interface

2. Getting Started

The CDI Optical Spectrometer has been designed for ease of installation and use. Since the optic is factory calibrated, you may begin data acquisition immediately after installing the instrument. A quick-start installation that uses the default, factory settings is outlined below.

a. Install the spectrometer card in the PC's ISA slot. If the spectrometer has a Universal Serial Bus (USB) interface connector, plug in one end of the USB cable to the available USB port on the PC computer and the other end of the USB cable to the spectrometer.
b. Install the CDI Spec32 software. (See software installation section)
c. Install the correct device driver corresponding to the spectrometer's interface
d. Double click the Spec32 icon on the desktop to start the program.
e. Connect the light source input fiber to the SMA connector and begin data acquisition.
f. Ensure the light source is turned on and the light path is unobstructed.
g. Optionally press the Auto Configure button to tune in the signal automatically. This configures the exposure time (integration time) to sample 50,000 raw A/D counts, if possible.

3. Hardware Installation

Spectrometers with an ISA Interface

The spectrometer card uses only the XT I/O bus for communications with the CPU. Interrupts and DMA channels are not used, simplifying the installation. The board address is preset at the factory. You may need to check your computer for I/O address conflicts. If another board is already using this address, use the procedure in the section on board address for resetting the spectrometer board address.

The optical spectrometer card will in most cases obscure the adjacent ISA slot, rendering it unusable. Make sure to remove the bulkhead cover from the adjacent slot to allow air intake for heat dissipation.

Spectrometers with a USB interface

Your spectrometer is shipped to you with a USB cable. Plug one end of this cable to a PC computer and the other end into the spectrometer, **Figure 3.1**. The location of the USB port can either be in the front panel, or in the back panel of the computer. The USB interface was designed as a hot-swappable interface, which means that the a spectrometer with a USB interface can be installed and used without having to power down the computer or the

spectrometer. (**Note: If your computer does not have the CDI Spec32 software package already installed, please turn off the power of the spectrometer before plugging the USB cable into the computer).**

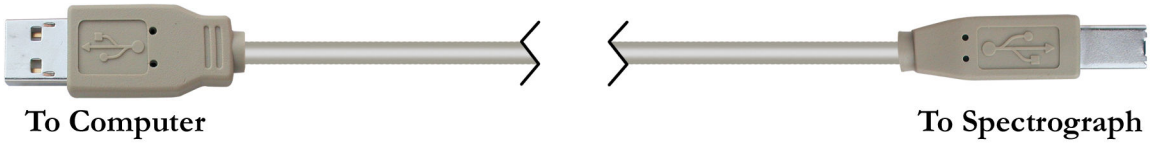


Figure 3.1: USB cable

CAUTION

You need to have Administration Privileges in order to install and modify software and hardware under Windows NT/2000/XP/Vista

CDI SPEC32 CDI-Rom Disk

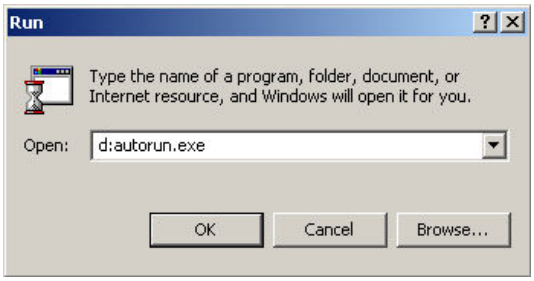
4. CDI Spec32 Software installation under Windows 9x, ME, XP, NT, and 2000, and Vista

A CD-Rom disk is shipped with each spectrometer, depicted in **Figure 4.** This CD-Rom disk contains CDI Spec32 software, this manual in PDF format, and other useful documents. Installing CDI Spec32 software is straightforward and simple. Follow the steps below. Up to date Spec32 software packages can be obtained from the CDI website as well.
Visit http://www.controldevelopment.com/downloads/

4.1. Insert the CDI Spec32 CD into the CD-Rom drive. It will automatically run and a menu comes up, **Figure 4.1.** If the Control Development **Main Menu** does not display, click **Start** button on Windows taskbar, and click **Run.** Type D: autorun.exe (where D is the letter corresponding the CD-Rom drive) in the Run Open box. **Figure 4.2.**

Control Development Main Menu

4.2. There are six choices to choose from on the **Main Menu**. You can either click on **View CDI Manual** (this manual you are reading) or **View CDI Catalog** for CDI latest products. Click on **Exit** will close this menu. To install CDI Spec32, click on **Install CDI Spec32 V…** option. Answer "Yes" to install CDI spec32, or "No" to exit to the main menu.



Run Open Box

4.3. A software compatibility matrix window displays, **Figure 5.1.** After you finish reading this table to confirm if your operating system is compatible with CDI SPEC32 software, click **OK.** (Please read the section 5 for more information about the software compatibility matrix.)

4.4. It is strongly recommended that you need to exit all Window programs before continuing the installation process of this program. The CDI SPEC32 software setup begins and a welcome screen displays, click **NEXT.** A Software License Agreement Window comes up. If you agree with Software License Agreement, click **YES** to continue the installation.

4.5. After you click **YES,** a software version release note displays. This is the information of the version of the program. If there were any bugs fixed from previous versions, or new features added and new release date of the program, they are listed here on this **Readme Information Window**. You can scroll left, right or up and down to see all information inside of this Window. Click **NEXT** to continue.

4.6. Enter your name and company name in the User Information Window, and click **NEXT.** As a default, CDI SPEC32 is installed in the CDI32 folder in C: drive. You can also install CDI SPEC32 in any folder or directory and drive by clicking on the **Browse…** and then select drive letter and type in or select the folder that will be used to install the program, then click **OK.** Click **NEXT** to continue the installation. **Note:** If CDI Spec32 is installed in a different folder then its default folder, the 8.3 file format rule must be followed. All folders CDI Spec32 is installed in must have 8 characters or less includes the CDI Spec32 folder. **It's highly recommended to use all default settings to simplify the installation and avoid complications.**

4.7. Select a Program Folder or use the default setting "**CDI Spec32**". Click **NEXT** will take you to the next Window where it displays all of the information you have typed in. You can always click on **BACK** button to go to previous pages to fix any mistakes. When you are ready, click **NEXT** and setup program will start copying necessary files to the computer. This process may take up to several minutes, depending on the speed of the computer.

4.8. When the setup program stops, a Setup Devices Windows displays, **Figure 4.3**. Depending on the operating system, this screen might be slightly different. Click **OK** on this Windows, and then click **OK** again to finish the installation. You will then be asked to restart the computer. Please restart the computer before using this program.

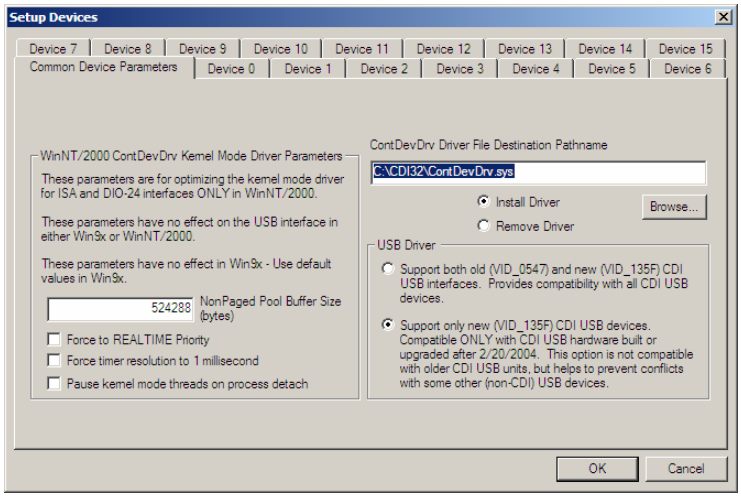


Figure 4.3: Setup Devices display. Up to 16 devices can be setup and run simultaneously

5. CDI Spec32 Software Compatibility Matrix table

	Operating System				
Interface	Windows 95	Windows 98/SE/ME	Windows NT	Windows 2000/XP	Windows Vista
ISA Plug-in Card	Spec(16-bit) Or Spec32	Spec(16-bit) Or Spec32	Spec32	Spec32	Not Supported
DaqCard DIO-24 (PCMCIA bus)	Spec(16-bit) and NiDAQ Ver 5 (16-bit) Or Spec32 and NiDAQ Ver 6.x	Spec(16-bit) and NiDAQ Ver 5 (16-bit) OR Spec32 and NiDAQ Ver 6.x	Spec32	Not Supported	Not Supported
PC-DIO-24 (ISA bus)	Spec(16-bit) and NiDAQ Ver 5 (16-bit) Or Spec32 and NiDAQ Ver 6.x	Spec(16-bit) and NiDAQ Ver 5 (16-bit) OR Spec32 and NiDAQ Ver 6.x	Spec32	Spec32	Not Supported
PCI-6503 (PCI bus)	Spec32 and NiDAQ Ver 6.x	Spec32 and NiDAQ Ver 6.x	Spec32	Spec32	Not Supported
USB Interface	Spec32 (Win95 with USB Supplement)	Spec32	Not Supported	Spec32	Spec32

Figure 5.1: CDI Software Compatibility Matrix Table

CDI Software Compatibility Matrix table, **Figure 5.1** is a chart that shows the compatibility between CDI hardware interfaces, CDI software and the operating systems.

Example 1: If you run a CDI spectrometer with USB Interface in Windows 98, look at the chart where it says **USB Interface** on the first column. Move across to the third column where it says **Spec32**, and the header in the second row of that same column says **Windows98/SE/ME**. That means SPEC32 software will be compatible with USB Interface, and Windows 98/SE/ME operating systems support USB interface.

Example 2: If you would like to run a USB interfaced spectrometer in Windows NT, you will find out that your spectrometer with USB interface will not be compatible with Windows NT. By looking at the chart where it says **USB Interface** in the first column. Move across until you get to the fourth column where it says **Not Supported** and the header in the second row of that same column says **Windows NT**. That means there is no CDI software support USB interfaced spectrometers in Windows NT operating system. **Windows NT does not support USB interface.**

6. Setup Device Driver

By this time, you should have already installed CDI Spec32 program on your computer and either installed a spectrometer with ISA, or USB interface or both.

If you installed a spectrometer with ISA interface, you are ready to setup the device driver for that spectrometer. **Note:** If you installed more then one ISA interfaced spectrometers, or have problem with board address confliction, please see section Board Address Setting. If you installed a spectrometer with USB interface, turn on the power switch of the spectrometer. It may take up to a few minutes for the operating systems to install the USB device driver for the spectrometer. Before we move on to the next step, lets take a look at the LED lights on the front panel of the spectrometer, and what they mean.

6.1. L.E.D. Indicator Lights On The Spectrometer, what do they mean?

There are three L.E.D. (Light Emitting Diode) indicator lights on the front panel of the spectrometer with USB interface: Red, Orange, and Green.

6.1.1 Red LED

The Red L.E.D. is the spectrometer power indicator light. When this light is on, it means the spectrometer main power is turned on.

6.1.2 Green LED

The Green L.E.D. is the USB indicator light. When this light is on, it means the USB cable is connected to the computer and the spectrometer, and the computer is running. This Green L.E.D will stay on regardless if the spectrometer main power is on or off as long as the computer that connects to the spectrometer is on.

6.1.3 The Orange L.E.D. can indicate three different situations

6.1.3.1. When this Orange L.E.D. is off, even if the spectrometer and the computer power are turned on; it means there is no communication between the computer and the spectrometer. **You may not have installed CDI Spec32 program on the computer, or the USB port was not installed properly. Please consult the USB manufacture's instruction manual.**

6.1.3.2. When this Orange L.E.D. is dimly blinking, it means there is communication between the spectrometer and the computer. CDI Spec32 software and device driver for USB were installed properly. **Note: For spectrometers running USB 2.0 HiSpeed firmware, the Orange L.E.D. will only blink until the first data access. That would consist of either reading setup data from flash or reading a spectrum.** Now you can proceed to setup device driver for the spectrometer in the S**ection 6.2**.

6.1.3.3. When this Orange L.E.D. brightly blinking, it means that the spectrometer and the computer are exchanging data. This only happens when taking

samples with the spectrometer. Once the acquisition finishes, the light will turn off.

6.2. CDI Driver Installer Program

Before a spectrometer can work with CDI Spec32 program, it must have a particular device driver installed. A **CDI Driver Installer** program that was installed together with CDI Spec32 program will simplify this task. By running **CDI Drive Installer** program, you will then be able to setup the device driver and access different parameters of each spectrometer.

6.2.1 Run CDI Driver Installer Program

Click **Start** button on Windows taskbar, then choose **Programs** and look for CDI Spec32 on the slide-out menu, then click on **CDI Driver Installer**. After the **CDI Driver Installer** started, a **Setup Device Driver** screen displays, **Figure 6.2.1.** This screen is slightly different from one operating system to another.

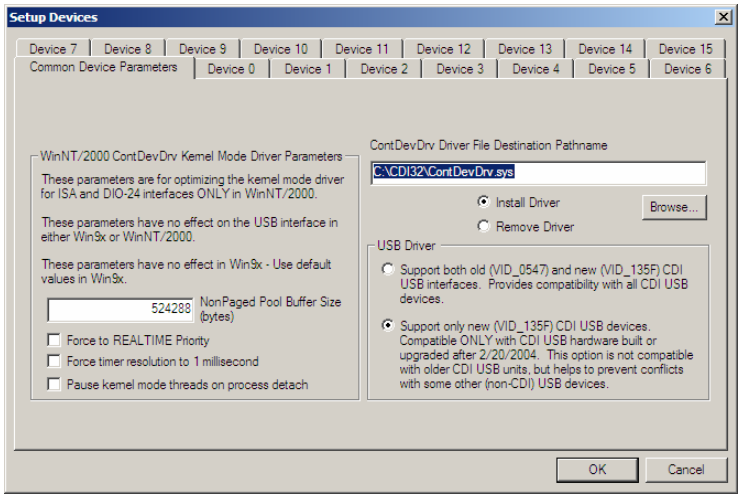


Figure 6.2.1: Setup Devices for Windows NT, XP and 2000
Up to 16 spectrometers can be installed and run simultaneously

6.2.2 Common Device Parameter Screen

The Setup Devices main screen is Common Device Parameters. This is a default screen. Every time the CDI Driver Installer runs, this screen will be displayed. There are also 16 identical Setup Device screens, labeled as Device 0 to Device 15. These setup device options are where you can specifically choose the correct device driver for the interface types of the spectrometers installed, and other important parameters.

6.2.2.1. ContDevDrv Driver File Destination Pathname

The pathname, C:\CDI32\ContDevDrv.sys, is the default pathname to the ContDevDrv.sys file. This pathname can be different, depending on the location where CDI Spec32 was installed. Regardless of whether the operating systems are running, the pathname to the ContDevDrv.sys has to be displayed in this text box. If this text does not display the pathname to ContDevDrv.sys, you can either type it in or use the **Browse** button next to the text box and locate the ContDevDrv.sys file.

6.2.2.2. Install Driver and Remove Driver

There are two radio buttons below the text box. One labeled **Install Driver**, and the other labeled **Remove Driver**. They mean exactly what they are labeled. When the **Install Driver**'s radio button checked, the device driver will be installed. When the **OK** button is clicked, **Setup Devices** window will be closed, and a small window displays, "Driver successfully installed". The default is **Install Driver** checked.

To remove the device driver, click on **Remove Driver** radio button, and all of the device driver will be removed when the **OK** button is clicked, **Setup Devices** window will be closed, and a small window displays, "Driver deleted from registry". **Note:** If the device driver is removed, all of the spectrometers will not have communication with CDI Spec32 until the **Install Driver** radio button option is checked, and the device driver installed again.

6.2.2.3. WinNT/200 ContDevDrv Kernel Mode Driver Parameters

6.2.2.3.1. Win9x and ME

These parameters are slightly different from one operating system to another. These parameters are grayed out in Win9x, ME, which means these parameters cannot be changed, and default will be used

6.2.2.3.2. WinNT, 2000, and XP

These parameters are for optimizing the kernel mode driver for ISA and DIO-24 interfaces. These parameters have no effect on USB interface regardless of the operating systems. The default values parameters are listed below:

- Text box, **NonPagedPool Buffer Size [bytes] = 524288**
- ☑ **Force to REALTIME Priority, checked**
- ☑ **Force time resolution to 1 millisecond, checked**
- ☐ **Pause kernel mode threads on process detach, unchecked.**

6.2.3 Device 0 to Device 15 Tabs

A total of 16 spectrometers can be installed and run simultaneously by CDI Spec32 as long as the correct device driver is selected and installed for each spectrometer. **Note: The more spectrometers are installed on a computer, the more CPU time they take to run. Take this in consideration when planning on installing more than one spectrometer.**

Different interface types can be installed, mixed and matched in CDI Spec32 if they are installed in the order from Device 0 to Device 15. Device 0 must be installed first before Device 1 can be installed. Device driver can be installed ahead of time without an actual spectrometer plugged in. The reason for this is when a spectrometer is plugged in at the later time, you don't have to install the device driver again

Click on the tab labeled **Device 0** so it will be active, and the setup device screen looked similar to **Figure 6.2.3.** Remember, this screen is slightly different from one operating system to another. There are several parameters on the Device 0 page. Depends on what operating system and the interface of the spectrometer installed, these options are either enabled or disabled.

6.2.3.1. Interface Type

Select the correct interface type of the spectrometer installed. Click on the down arrow to the right of the text box. There are five different interface types to choose from the pulldown list. Depends on what interface type selected, that will enable or disable some of the parameter below.

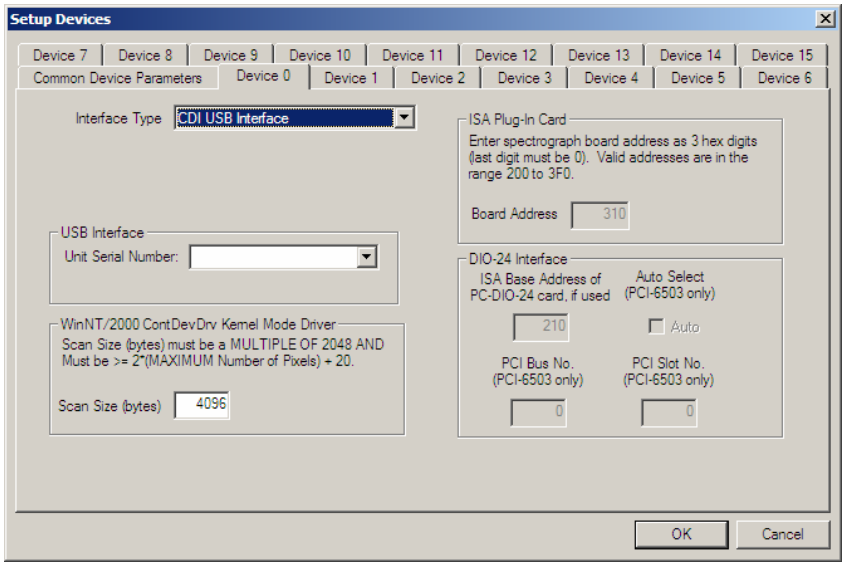


Figure 6.2.3. Device 0 setup screen active in Windows NT/2000

6.2.3.1.1. CDI Direct ISA Plug-in

CDI Direct ISA Plug-in is for spectrometer with ISA interface. This type of spectrometer is normally plugged in the 16 bits bus slot inside the PC computer. If this interface type selected, all of the parameters below it would be grayed out except where it says. **"**ISA Plug-in Card", **Figure 6.2.3.1.1a** and **Figure 6.2.3.1.1b**

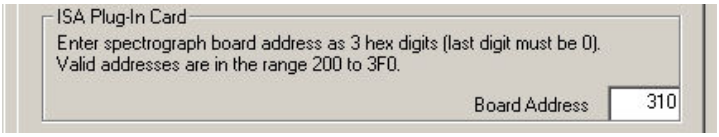


Figure 6.2.3.1.1a: ISA plug-in card board address Option

The default value of the Board Address is 310. Enter the correct board address by to the setting board address of the ISA spectrometer as 3 hex digits. The last digit must be 0. Each ISA interface spectrometer has its own, unique board address. If more than one spectrometer is using the same board address, there will be a board address conflict. Please refer to Board Address Setting in the next section to find out more about how to set board address for each spectrometer.

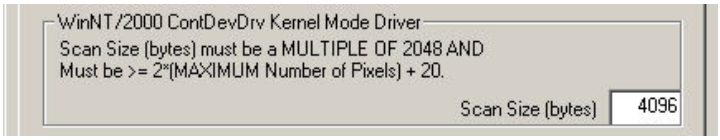


Figure 6.2.3.1.1b: This parameter is only enabled in Windows NT/2000/XP

WinNT/2000 ContDevDrv Kernel Mode Driver parameter is for optimizing memory setting. The default is set at 4096. It is strongly recommended to use this default setting to avoid any complication that might occur.

Note: The WinNT/200 ContDevDrv Kernel Mode Driver parameter is always enabled in Windows NT, 2000 and XP, regardless of the selected interface type. This parameter is always grayed out in Windows 9x,ME, and the default value is used. Always click on **OK** button when you finish.

6.2.3.1.2. Nat. Inst. PC-DIO, ISA

Nat. Inst. PC-DIO, ISA (National Instrument PC-DIP,ISA) is an interface that connects the PC computer to an external spectrometer such as MPP, NIR or Raman spectrometer via a cable. If this interface is selected, the DIO-24 Interface parameter is also enabled, **Figure 6.2.3.1.2**

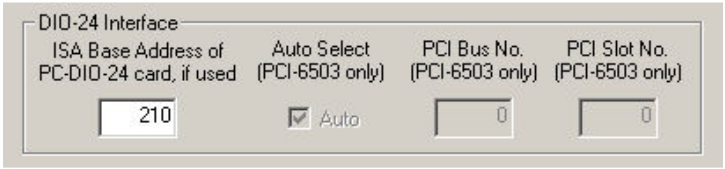


Figure 6.2.3.1.2: DIO-24 Interface ISA Base Address setting enabled

The default Base Address of PC-DIO-24 ISA card is 210. Enter the correct Base Address corresponding to the PC-DIO-24 ISA card that is installed in the computer. Make sure that this Base Address is not being used by any other hardware in the computer, or if more than on PC-DIO-24 ISA cards installed in the same computer, they should all have different Base Address settings. Please consult the National Instruments instruction manual.

6.2.3.1.3. Nat. Inst. PCI-6503, PCI

Selecting the Nat. Inst. PCI-6503, PCI will also enable the DIO-24 Interface parameter, **Figure 6.2.3.1.3.**

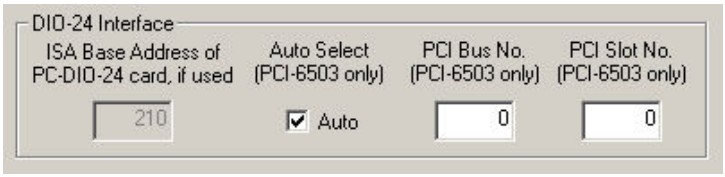


Figure 6.2.3.1.3: Default setting for Nat. Inst. PCI-6503, PCI

When the Auto check box is checked, the Device installer will automatically detect the first PCI-6503, PCI board and assign it as Device 0. There is special a situation where there is more than one board of the same type installed and used for other instruments rather than CDI Spectrometers, then the PCI Bus No. and PCI Slot No. must be given so they can identify which is CDI Spectrometer, and which is not.

6.2.3.1.4. Nat. Inst. DaqCard DIO-24, PCMCIA

Nat. Inst. DaqCard DIO-24, PCMCIA interface is normally a plug-in interface for Laptop computer to operate a spectrometer connected via a cable. There is no editable parameters when this interface is selected. **Note:** Only one Nat. Inst. DaqCard DIO-24, PCMCIA interface can be plugged in and used one at a time.

6.2.3.1.5. CDI USB Interface

Selecting The CDI USB Interface will also enable the USB Interface Unit Serial Number, **Figure 6.2.3.1.5.** **It is recommended to leave this text box blank if only one spectrometer will be used at a time with this PC, which is by far the most common scenario.** Click the down arrow to the right of the text box and select the serial number of the spectrometer that you would like to install the device driver for. When finished, click **OK** to install.

Figure 6.2.3.1.5: This box will only be enabled when a USB Interface is selected

Leave the Unit Serial Number blank when a single spectrometer is installed on the PC. Do not select or type in the unit serial number unless you are installing more than one spectrometer using multiple device number tabs (Device0, Device1, etc).

6.2.3.1.6. CDI USB 2.0 HiSpeed Firmware

In late 2008, CDI introduced a new firmware revision designed to work with USB 2.0 High Speed ports and controllers. The firmware takes advantage of the faster speed of the USB 2.0 interface and now allows for arbitrarily large buffer (FIFO) size in software rather than hardware. (The buffer can fill with up to 2048 samples.) It also takes less time to start an acquisition [.25 ms], so in general it is faster than any previous USB firmware.

To ensure proper installation of the HiSpeed firmware follow these instructions.

NOTE: The following procedure is only required for USB 2.0 spectrometers delivered before the HiSpeed firmware release (Spec32 version 1.7, January 2009). All USB 2.0 units delivered after that time are factory pre-configured to run the HiSpeed firmware.

InstDrvGui.exe has been changed to update a word of the spectrometer's flash which causes the new USB2 driver to be loaded. To initialize the spectrometer, an up to date driver must be installed.

1) Run the installation (InstDrvGui.exe) without the spectrometer attached. If the spectrometer is attached at this time, it will hang up in InstDrvGui.exe and will require that the USB cable be disconnected to continue.

2) After installing the new driver, then run InstDrvGui.exe **again** with the spectrometer attached. This will allow InstDrvGui to update information in the internal flash memory using the new driver.

3) Finally, power cycle the spectrometer by disconnecting the power and USB cables. Then, reconnect those cables and the updated firmware will load.

Important: To check if your spectrometer is running with the USB 2.0 firmware, simply invoke the menu command Setup | Set Buffer Size and try to change the value in the dialog. If you pull the dialog up again and it has changed, the HiSpeed firmware is running.

The firmware will automatically downgrade to the older USB 1.0/1.1 firmware and speeds when faced with a 1.0/1.1 port, so backward compatibility is not an issue.

7. Special note for CDI Interface Kit

If you use CDI Interface kit that either has Nat. Inst. PC-DIO-24, ISA or Nat. Inst. PCI-6503, PCI interface build-in; change the board address of the ISA spectrometer card to 310 before plugging it in the CDI Interface kit. Select the Interface Type in the Setup Devices corresponding to the type of interface that is used in the CDI Interface Kit.

8. Calibration File Installation

Each spectrometer is shipped with a calibration disk. This floppy disk contains permanent wavelength calibration files and reference files. These files are unique and specially created at the factory for each spectrometer. Before a spectrometer can communicate with CDI Spec32, these calibration files have to be loaded to the computer memories. Also each spectrometer has flash memory where calibration file stored. With the new release CDI Spec32, these calibration files will be loaded to computer memories automatically.

7.1. Load Calibration File From Flash Memory

Begin CDI Spec32 version 1.22, there is a build-in feature that will detect and load calibration file from flash memory every time CDI Spec32 runs. Loading calibration file from flash memory will eliminate the classic way of copying calibration to computer hard disk. But if you still prefer the classic way, please follow the steps below.

7.2. Install Calibration Files For ISA Interface Spectrometers

7.3.2. Create a folder inside CDI Spec32 or where you have installed CDI Spec32
7.3.3. Name this folder same as the spectrometer serial number. For example: If your spectrometer's serial number is SNLC109, name the folder as SNLC109.
7.3.4. Insert the calibration disk in the floppy drive, normally drive A:
7.3.5. Copy all files from floppy disk to the folder you just created.

7.3. Install Calibration Files For USB Interfaced Spectrometer

1. Insert the calibration disk in the floppy drive, normally drive A:
2. Copy the folder (this folder should be the same as the spectrometer's serial number) from the floppy disk to the CDI Spec32, or where you have installed CDI Spec32.

8. Uninstall CDI Spec32

Uninstall CDI Spec32 is quick and simple. Click **Start** button on the Windows taskbar, and select **Control Panel.** When the **Control Panel** Window opens, select **Add/ Remove Programs**, when the **Add/Remove Programs** Window opens, select CDI Spec32 for Win 9x/NT/2000, and click on the **Remove** button. Follow the instruction given by your Windows operating system. Even though CDI Spec32 program is removed, all of your data that was saved in CDI Spec32 folder will still be safe.

9. Updating CDI Spec32

9.1. Updating CDI Spec32 From CD-ROM Disk.

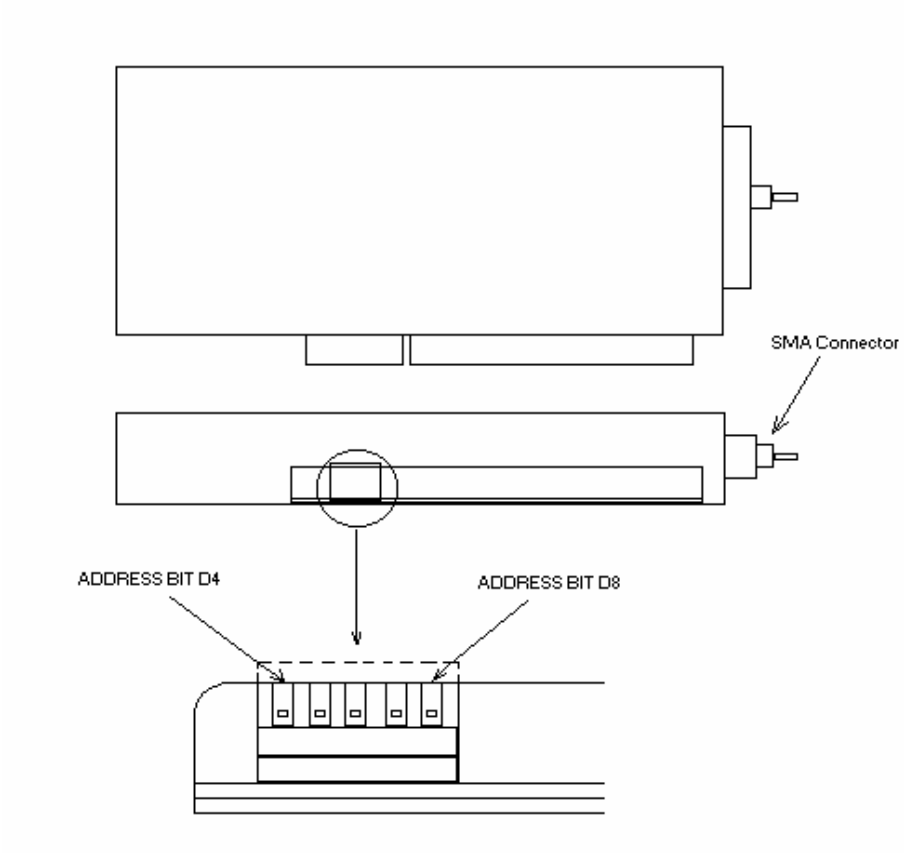
Please read Section 4.1 to 4.9, page 5 to update CDI Spec32 from CD-Rom. If you previously installed CDI Spec32 in a different folder other then the default folder, please remember to browse to that folder to install the updated version. The existing CDI Spec32 version will be over written by the updated version. The CDI Spec32 updated version will use the existing calibration files.

9.2. Updating CDI Spec32 With a Downloaded File From CDI Website

If you downloaded an updated version of CDI Spec32 from CDI Website, browse the folder where the update version CDI Spec32 is saved, double click on the file name and installation process begins. Please read Section 4.5 to 4.9, page 5 for more information. To download the latest update version of CDI Spec32, visit CDI website at http://www.controldevelopment.com/index.php?topgroupid=1&subgroupid=2&groupid=11

10. Board Address Setting

The ISA unit board address was set at the factory with the default setting of 0310 hex. This should allow for operation on most computers. However should you have an address conflict you can change the board address using the following information.



S1 S5

S5	S4	S3	S2	S1	reserved	Address (hex)
1	0	0	0	0	0000	300
1	0	0	0	1	0000	310
1	0	0	1	0	0000	320
1	0	0	1	1	0000	330
1	0	1	0	0	0000	340

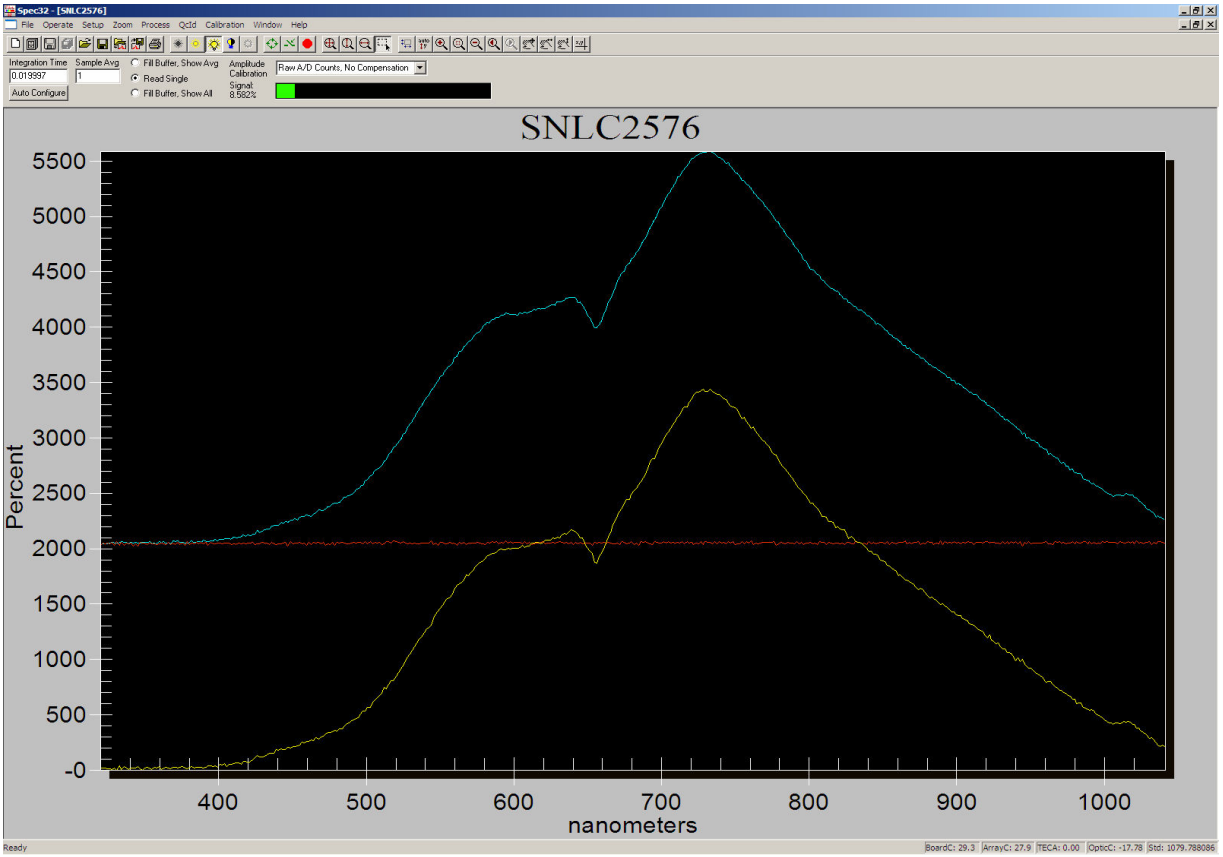
Switch up = on = 1
Switch down = off = 0

Chapter 2
CDI Spec32 Overview

The CDI Spec32 software is designed to give the user control over the instrument settings and the sampling parameters. To do so, many low level commands have been provided. Setting up the instrument for a given measurement requires some manual adjustments. These adjustments, however, only need to be done once for any given test. After that the setup can either be saved as a file for future use or will become the default setup and be loaded the next time the unit is turned on.

The setup files are also compatible with the driver function dynamic link library (DLL), the National Instruments LabVIEW® sub-VI node, and the ActiveX Control. This allows the user to create custom applications without providing complete user interfaces, instead using the SPEC application's GUI to create the instrument setup files.

Below is a sample of the CDI Spec32 screen. The following sections will give detailed descriptions of the different areas of this screen.



1. Menu Description

All available commands may be accessed from the menu. However, the most often used commands also have Toolbar buttons for convenience, and the most frequently used controls are also available from the control bar. The menu has been divided into sections using Windows API design guidelines. A general overview for each main menu entry is given below.

File	Standard file commands such as List Devices Connected, Open, Save, and Create Configuration; Open and Save Setup; Open and Save Setup from Flash; Open and Save Trace; Save and Print graphs; Open Kinetic Date and View Kinetic ASCII; Trace Log and Exit.
Operate	Where you can find spectrometer operating commands such as Scan Single, Scan Continuous, and Abort Scan; Shutter on/off, Store Reference and Background, Acquire BG, Acquire reference, Acquire Ref and BG, Auto Integrate…
Setup	All Setting commands for graphs and hardware are listed here: Trace Display, Trace Legend, Trace Data Table, Delete All Traces, Integration Time, Trigger Mode, Amplitude Calibration, Sample Averaging, Wavelength Interpolation, Graph Settings, Data Cursor On, High Priority GUI.
Zoom	There are all the standard view commands such as Zoom Default, Zoom Fit XY-Axes, Zoom Fit Y-Axis, Zoom Fit X-Axis, Zoom Settings… Zoom In, Zoom Out, Zoom Autoscale Y, Zoom Redo, Zoom Undo, Pan X, Pan Y, Pan XY.
Process	Data processing command such as Savitsky-Golay smoothing, Peak Detection,
Window	MID commands such as Toolbar, Status Bar, Cascade, Tile, Arrange icons, and List of Devices…
Help	About Spec32… (Provides version info)

2. Status Bar Description

The status bar displays messages, which indicate the activity of the instrument and status of the operation. The status bar also provides a convenient real-time text display of mouse coordinates and array temperature. The following is a snapshot of a typical status bar during operation.

The left area of the status bar is used to display **User Status Messages** and **Command Help Strings**.

2.1. User Status Messages

Include a sample counter, which indicates the status of a multiple [averaged] sample trace, a count down timer to indicate the time remaining to a completed sample, and the number of samples averaged, in the case of **Fill Buffer** mode.

2.2. Command Help Strings

Describes actions of menu items as you use the arrow keys to navigate through menus. This area also shows messages that describe the actions of toolbar buttons as you depress them, before releasing them. If after viewing the description of the toolbar button or command you wish not to execute the command, then release the mouse button while the pointer is off the toolbar button or menu item.

2.3. BoardC

This box displays the ambient temperature at which the spectrometer is operating in degrees Celsius. If the spectrometer is installed inside a computer rather than externally connected, this reading will be higher than it would otherwise be. The ambient temperature naturally will also influence the Detector Array temperature. The higher the ambient temperature is, the more the Detector Array's cooler has to work to keep the Detector Array temperature stabilized. All CDI spectrometers have a board level temperature sensor.

2.4. ArrayC

This box displays detector array temperature in Celsius. The lower the detector array temperature is, the more the detector array cooler has to work, and so more current will

be used. Some spectrometers may not have a temperature sensor on the detector, causing this reading to display meaningless values.

2.5. TECA

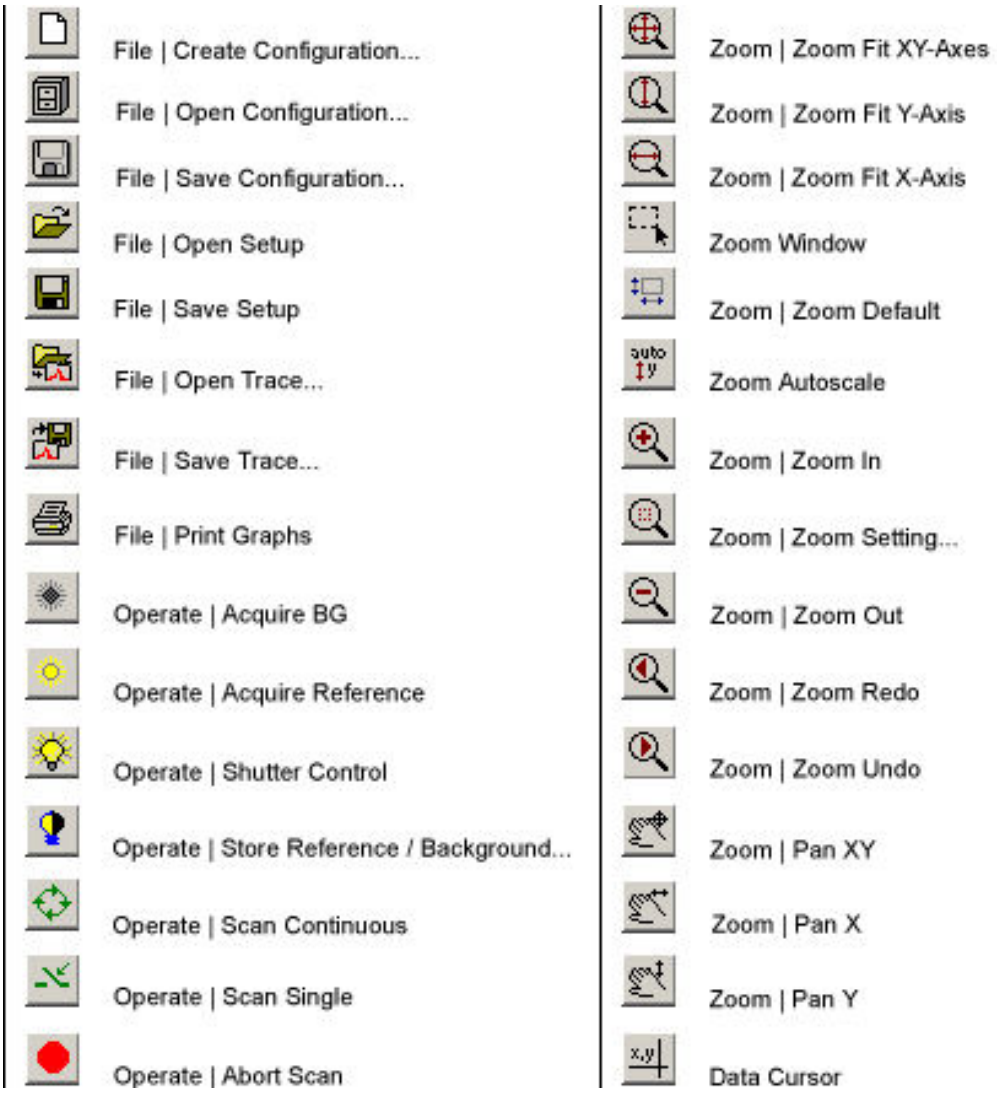
This box displays the current (in Amperes) of the detector array's thermoelectric cooler. This number will increase as the detector array cooler uses more current. When it gets to its limit, the detector array temperature will be out of range, and the spectrometer will not be able to hold temperature. In order to correct this, you either have to lower the ambient temperature, or raise the detector array temperature in the Hardware Settings. (See Hardware Settings, Chapter 5, Section 11).

2.6. OpticC

Displays the most recently sampled temperature of the optic temperature sensor in degrees Celsius. This will, of course, only return useful information if the optional temperature sensor is installed on the spectrometer. The "optic" in this context is the grating / mirror assembly mounted on top of the detector array. Some spectrometers have an optional temperature controller to stabilize the optic temperature, hence the need for the sensor.

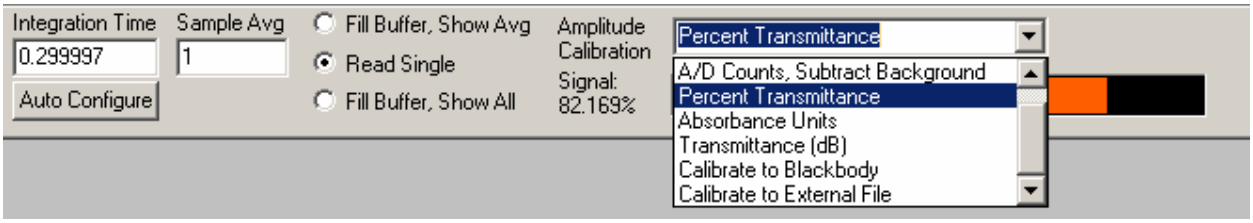
3. Tool Bar Description

The Toolbar provides icons push button control types. These buttons are actually short cut commands to the menu items listed below. When a mouse cursor moves over the button, a short description is displayed in the Control Tip Text box momentarily. The description will tell what the button will do when the cursor is over the button, and the left button is pushed and released.



4. Control Bar Description

Frequently used controls are included in the control bar located at the top of the screen. This control bar allows the user to update control parameters on the fly. The control bar provides all the controls required to quickly configure the spectrometer for a desired signal level. The items on the control bar are explained below.



4.1. Integration Time

Exposure time of the array. Signal level is proportional to integration time; that is, the longer the integration time, the larger the signal that is shown on the screen. In absence of light, a longer integration time will have only a slight influence on signal level.

4.2. Sample Avg.

This determines the number of samples that will be accumulated in an average. The signal-to-noise ratio increases as the square root of the number of samples averaged. The greater the number of samples taken, the less effect noise will have on the signal.

4.3. Fill Buffer, Show Avg

When this option is selected it causes the on-board FIFO memory to be filled, and the average is displayed on the screen. This can be used for increasing the acquisition rate for integration times shorter than 110 ms, due to the lower latency between each sample. Fill buffer is preferred whenever update time permits. Sample averaging **(4.2)** above can be used in tandem with this mode in place of using Read Single **(4.4)** with a higher number of averages. However, for units that are using a firmware prior to HiSpeed USB 2.0, the buffer size is fixed and typically holds no more than 8 spectra. If used together, the total number of samples averaged is the size of the buffer (in spectra) multiplied by the Sample Average parameter.

4.4. Read Single

When this option is selected the data is sent to the screen after each sample is taken as a single trace. This provides immediate visual feedback to help make configuration adjustments. This mode is almost as fast as the Fill Buffer mode for integration times greater than 110 mS.

4.5. Fill Buffer, Show All

This mode takes all the samples in the on-board FIFO memory and displays them when acquisition has finished. For example, for a unit with enough memory to store 32 spectra, this mode will cause 32 spectra to be acquired and then displayed on the screen. The spectra are visually differentiated by the color of their graph line.

4.6. Amplitude Calibration

This pull down menu allows you to select any of the calibration units on the fly. For example, you can switch to A/D counts to take a background, optimize the signal level, store a reference, and then switch back to **Percent Transmittance** or **Absorbance** mode.

4.7. Signal Level Gauge

This bar expresses visually the maximum number of raw A/D counts among all the data points in the most recently sampled spectrum. 0% represents saturating low, an error condition, and 100% represents saturating high, a potential error condition. The percentage is expressed as the largest count value divided by 65,000, then multiplied by 100. The Signal Level Gauge is useful for when one needs to work in compensation modes that don't utilize raw counts, enabling the user to know the signal level and adjust the integration time without having to switch back to a raw counts mode. (Raw A/D Counts and A/D Counts Subtract Background modes) Primarily, this gauge exists to help avoid saturating high during data acquisition. Low numbers of counts are expressed as green shades, midrange counts as shades of yellow / orange, and very high count values as red.

Chapter 3
Taking your first Trace

By this time, the spectrometer is installed, and a proper device driver has been selected for it. It's time to verify full communication with the device by taking the first trace. Start by turning on the computer.

If the spectrometer uses a USB interface kit with an on / off switch, turn it to the on position (or simply plug in the power supply, if applicable. The red and green LEDs should be on, and the orange LED should be off, if the USB cable is unplugged. If the USB cable is unplugged, plug it in and it should begin blinking. If the orange LED persists in staying turned off, verify that the USB cable is in fact connected directly to the PC. Lastly, contact CDI for tech support if the LED refuses to blink / illuminate.

If the spectrometer uses an ISA interface, the unit should already be receiving power over the edge connector it is installed into. The red and green LEDs should be illuminated, and the orange LED should be flashing.

Note: Current firmware, including the USB 2.0 HiSpeed firmware, causes the orange LED to stop flashing after the first USB access, such as reading from flash. However, the LED should still flash after the power has been cycled, as well as when the PC accesses the spectrometer to read or write data.

1. What else will you need?

An SMA-to-SMA adapter is required to connect an optical fiber to the spectrometer if it is an ISA plug-in card, and a proper sized fiber. If the application requires taking data from wavelengths below 350 nm, a "High OH" cable is required; for wavelengths above 350 nm, use a "Low OH" cable. Connect one end of the fiber to the spectrometer and the other end to the light path / source to be used in data acquisition.

2. Run CDI Spec32 Program

Click the **Start** button on the Windows taskbar, then choose **Programs** and look for **CDI Spec32** on the slide-out menu, then click on **Spec32.** Spec32 will try to detect the spectrometer and load the setup file from flash memory. If everything goes well, then the default CDI Spec32 window comes up, **Figure 2.1,** else you will an error window, **Figure 2.2**. Please follow the instructions on the error box and retry again.

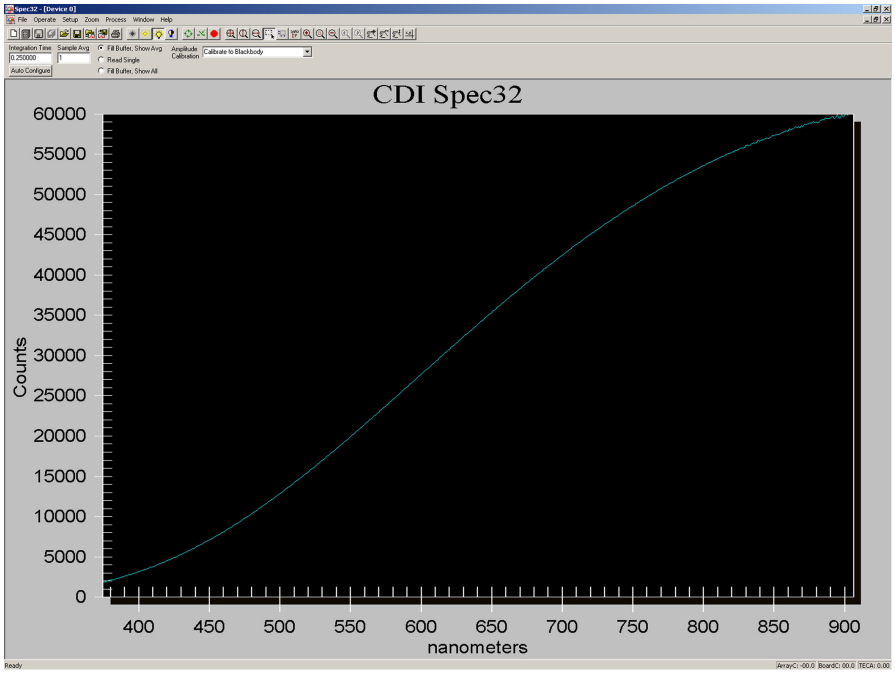


Figure 2.1 Default CDI Spec32 Windows

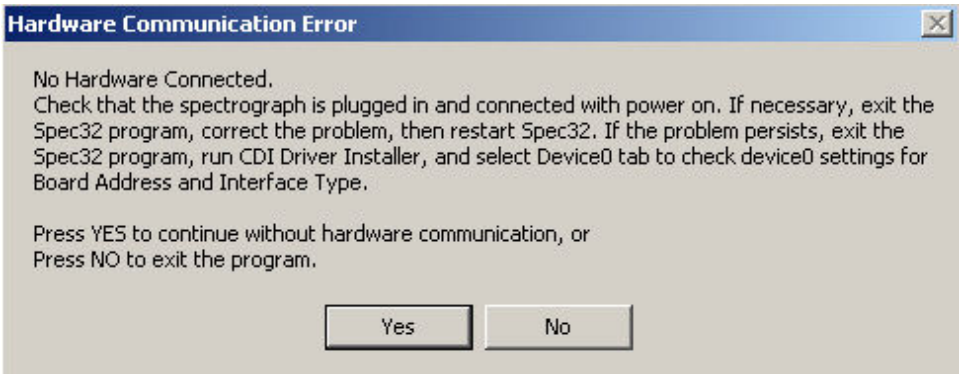


Figure 2.2 Hardware Communication Error

Note: It is advisable to let the spectrometer and accompanying light source run for 15 minutes prior to the beginning of sampling so that their temperatures can stabilize.

3. Auto Configure

The Auto configure button is a shortcut command to a pull down menu command, **Operate | Auto Integrate**. **Auto Configure** will attempt to determine a suitable the integration time for the spectrometer by gathering information from the intensity of the light source. It automatically adjusts the integration time until a signal level of about 50,000 counts is achieved.

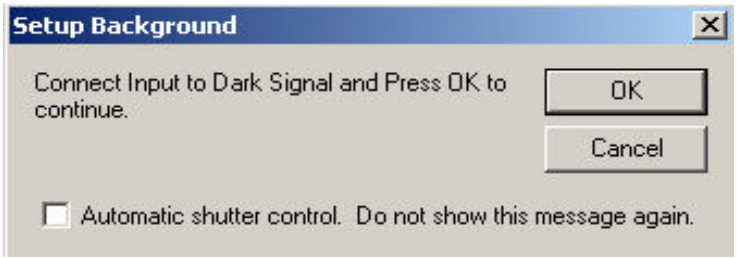
After clicking on the **Auto Configure** button, a prompt will appear asking to turn on the light source and then click on the **OK** button. It is recommended to use this command to set the reference integration time. The integration time can also be set manually by entering it in the **Integration Time** box.

4. Acquire Background

Next, a dark current signal, also called a background, should be obtained. This samples and stores the zero (dark) level for each wavelength. After clicking on the icon  on the toolbar, or accessing the menu command **Operate | Acquire BG,** a **Setup Background** dialog box comes up which prompts you to connect the input fiber to a dark signal, **Figure 4.1**. Covering the sample end of the optic cable with a cap or some other dark object in order to stop the light from entering the cable, then click **Ok** to continue.

Note: If you are using a CDI light source that has a shutter cable connected to the spectrometer, you can check the check box in the **Setup Background** dialog box labeled "Automatic shutter control, don't not show this message again." This will automatically turn the light source on and off when acquiring a background or reference.

The Acquire Background process will take a few seconds. When it's done, it will return to the main Spec32 window. The background that was just acquired is automatically stored as the "internal" background.



The Setup Background Dialog Box

Save Internal Background.

5. Acquire Reference

Next, an internal reference is needed. Uncover the fiber and expose it so that the maximum light that will be available to the sample. Some units may require a neutral density filter or other type of filter in the light path to prevent the detector array from saturating high. Click the icon  or use the menu item **Operate | Acquire Reference.** A dialog box will appear and prompt for the fiber to be connected to the light source. If using a light source connected with automatic shutter control built in, check the checkbox at the bottom of the dialog, which is pictured in **Figure 5.1**. Acquiring a reference will take a few moments depending on the current integration time. When it is done, it will return control to the main Spec32 window.

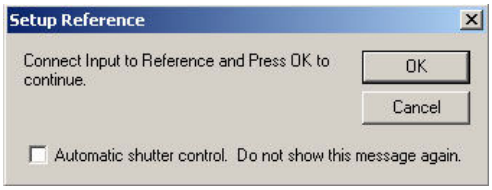


Figure 5.1 Setup Reference

6. Manually Storing a Background or Reference

If desired, one can store the current trace (the trace that updates after each acquisition) as a background or reference manually. To do so, click on the  icon or to use the menu command **Operate | Store Reference / Background**. The dialog box pictured in figure 6.1 will appear. Select the desired action**.** If storing a reference, by default the check box **Re-Compute Amplitude Compensation** will also be checked. Click **OK** to finish storing the trace.

Figure 5.2. By the default, the Re-Compute Amplitude compensation check box is also selected when the Store Internal Reference radio button is selected.

7. Automatic Procedure for Acquiring Reference and Background

All CDI Spectrometers come with an RJ45 connector on the front panel or on the end of the spectrometer card. This connector provides a way to interface the spectrometers to external accessories using CDI Spec32. See the **Pinout** section in **Appendix B**.

If you purchased a light source from Control Development Inc., then it has this interface built in. Connect the light source to the spectrometer via a RJ45 cable that was shipped with the light source.

Next select **Operate | Acquire Ref and BG** from the menu bar. This will take several seconds, depending on the integration time selected. When it finishes, control will return to the main window. The Reference and the Background were acquired and saved without user intervention.

8. Taking a Sample

The fiber should still be connected to the spectrometer, as well as the light source being on.

Place the sample in the light path and click on the  icon from the tool bar or access the menu command **Operate | Single Scan** and observe the newly acquired spectrum on the screen

To enlarge the spectrum so that the coordinate limits form a tight rectangle around the graph, click on the **Zoom Fit XY** icon  and the graph will be scaled accordingly. Please note that the zoom commands do not affect the range of wavelengths included in the sampling process; they merely view the data at different scales and positions.

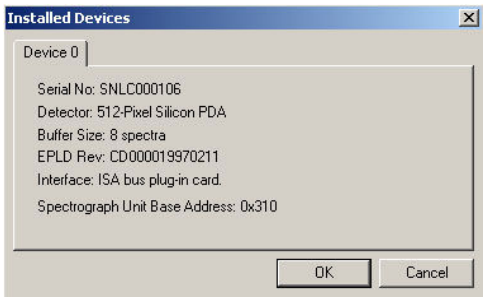
If **Zoom Fit XY** command zooms too far out, causing severe loss of viewable detail, the  and  icons can be used to tailor the coordinate limits. Also, one can also zoom in on a part of the graph by clicking and holding on a point and then dragging the mouse. The enclosed region will be rescaled to become the full graph window.

9. Saving Data

For the purposes of this tutorial, we will now describe only one of the simplest ways to save spectrometer settings and spectral data. Simply click on the save icon from toolbar  which is the same as the menu command **File | Save Setup**, and choose the location on the computer where the setup file will be saved. The **File | Save** Menu is described in detail in the next chapter.

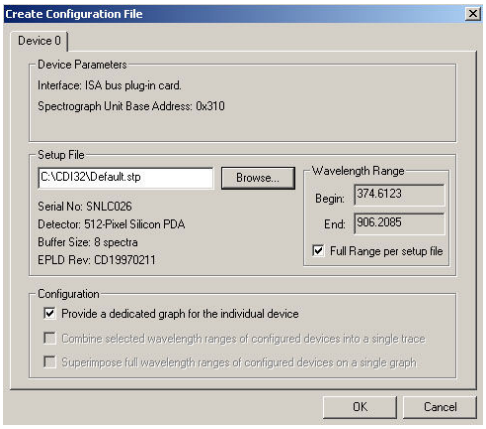
Chapter 4
Using File Command Menu

Select **File** from the menu bar, you will be able to access file commands. The capability to store and retrieve complete instrument setups tailored for various test and applications are some of the most powerful commands of CDI Spec32.



1. File | List Devices Connected

Use this command when you would like to know what type of the spectrometer or how many spectrometers are currently connected. The detector, interface type, unit serial number, and the board address can be found by using this command, **Figure 1.1.**



2. File | Create Configuration…

Use this command to create special setups of spectrometers and have that configuration opened automatically every time when the CDI Spec32 program runs. When run the **Create Configuration…** command, a **Create Configuration File** dialog box displays, **Figure 2.1.** If there is more than one spectrometer connected to the same computer, they will be shown in this dialog box, labeled from Device 0, Device 1 and so on.

2.1. Device Parameter

This tells you the type of the interface and the unit base address or (Board Address)

2.2. Setup File

Click on the **Browse** button to go to setup file location to select it and click open. After the setup file is opened, the actual wavelength range is displayed in the text box under **Wavelength Range**. Click on the check box where it says, **Full Range per setup file**. Check this if you want to use the actual wavelength range or uncheck it to edit the **Begin** and **End** wavelength range. A valid path to the setup file is required.

2.3. Configuration

If there is one spectrometer connected, only the first option will be enabled, and the other two options will be grayed out.

☑ Provide a dedicated graph for the individual device.
When this option is selected, an individual graph window will be given to every spectrometer that is currently connected and running in CDI Spec32.

Note: This option has to be checked if only one spectrometer connected.

If running multiple spectrometers, the two following options will be available.

☐ **Combine selected wavelength of configured devices into a single trace.**
When this option is selected in multiple units mode, CDI Spec32 will combine all traces of all spectrometers that currently connected, and run in CDI Spec32 into a single trace graph. This is useful when a single spectrometer alone lacks the wavelength range to view the entirety of a sample. The graph will splice the data from each wavelength range together into one continuous trace.

☐ **Superimpose full wavelength ranges of configured devices on a single graph**
When this option selected in multiple units mode, CDI Spec32 will superimpose all traces of all spectrometers that currently connected, and run in CDI Spec32 into one graph.

Note: All three options can be selected at the same time when running multiple spectrometers.

Click the **Ok** button, which will bring up a prompt to enter a file name in the **Save File** dialog box to save the configuration that you have just created. Enter the desired file name and click the **Save** button to finish.

Note: The default configuration file name is **setup$1.txt**. Please do not use this file name to save your configuration. CDI Spec32 overwrites this file name regularly. Use a descriptive file name that has something to do with the sample you are taking or serial number of the spectrometer that you are using.

In order to open the configuration automatically when CDI Spec32 runs, you have to use the **File | Open Configuration…** or **Ctrl + O** command and browse to the folder of your configuration file and open it manually at least once.

3. File | Open Configuration…

Use this command to load a configuration that you have created and saved. Click on **Open Configuration** from menu bar, you will be prompted to enter the file name. Configuration file

has the extension txt. Select the appropriate configuration file from the **Open Configuration File** dialog box and click **Open**.

Note: CDI Spec32 detects the unit serial number from flash memory every time it runs, and if you try to open a wrong configuration file, you will get an error message. Click **OK** and open a configuration file that is known to you.

4. **File | Save Configuration…**

   Saving configuration will save everything about the spectrometer that currently connected and run, including unit serial number, name of the setup file, and the graph. Click on **Save Configuration** from menu bar, and you will be prompted to enter file name with extension **TXT. Note: Do not use the default file name "setup$1.txt file. CDI Spec32 overwrites this file regularly.**

5. **File | Open Setup**

   Open setup file with extension **.STP** will load all the setup information of a particular spectrometer that was previously saved. The last instrument setting and the last data sampled, including the Reference and Background, Integration Time will be loaded into the computer memory. In the **Open Device0 Setup File** dialog box, select the setup file and click **Open.** If you try to open a setup file that was saved under a different spectrometer, you will get an error message.

6. **File | Save | Save Setup**

   This command saves the STP file, the most recently sampled trace in ASCII format, and the associated binary files. This command does not save the display, only the instrument settings and the last data sampled, including the Reference and Background.

7. **File | Open Setup From Flash…**

   The spectrometer is shipped with permanent wavelength calibration files and reference files stored in flash memory resident on the spectrometer module. This factory calibration may be loaded using this command. Open a setup file from flash by accessing to file menu and select **Open Setup From Flash**. A window comes up prompting you to select the Factory calibration file location, **Figure 7.1.** There may be several selections available, depending on the type of spectrometer and the version of the flash data format. Factory Calibration 1's radio button is always available and is selected by default. Selecting Factory Calibration 1 will let you load the calibration setup file that was saved at the factory before the spectrometer was shipped to you. Select the radio button of the calibration to load click **OK**.

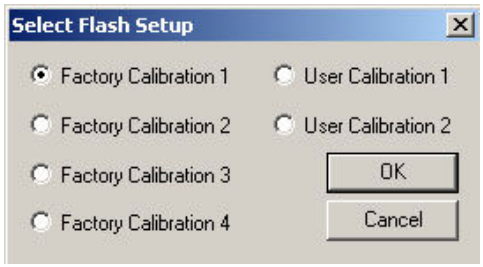


Figure 7.1. Open or Save Setup From Flash.

8. File | Open Trace…

Trace files saved using **File | Save Trace** have the extensions .DAT, .SPC, or .G00. Trace files saved as part of the setup file using **File | Save Setup File** are ASCII format with numeric extensions beginning with .0.

8.1. DAT Trace Files

Trace files with extension .DAT are ASCII (ANSI) encoded text files, which contain exactly one completely processed spectrum per file. The spectral data is divided into two columns: The left column contains the wavelength, and the right column contains the spectral data for that wavelength. Optional ASCII headers may also be stored inside the Trace file containing Instrument Setting or the trace headers may be stored without the spectral data.

8.2. SPC Trace Files

SPC files are encoded as binary files, and thus cannot be easily inspected of their data without special software. The file format was designed by Thermo Scientific (formerly Galactic and ThermoGalactic) for use with their software products. Most CDI software products can create and load SPC files as a matter of convenience for customers that need to do data acquisition using Thermo Scientific software and CDI software in conjunction.

8.3. g00 Trace Files

Also known as the "**Binary**" format, g00 files are collections of multiple traces combined into one file. The data is stored in a proprietary binary format that differs from the **SPC** format above. File names of the form "*.g*" are also recognized as Binary trace files in file dialogs, not just "*.g00" file names.

8.4. ASCII Trace Header Data

Additional metadata may be saved with the spectral data in the optional ASCII trace headers. Header options are provided for storing the Instrument Settings, Peak Detection results, Colorimetry results, and Prediction results. Multiple headers may be saved with the trace. The following is an example of the "Instrument Settings Header" and some truncated spectral data.

```
**Header1 Sampling Parameters**
TraceFile    C:\CDI32\Device 0_Trace 0.dat
Comment
Date   6/9/2009
Time   10:31:04
File Created By    CDI Spec32.exe
Software Version   1,7,0,6
Username     Bill
Computername BillsDELL
DeviceNum    0
SerialNo     SNLC02579
SetupFile    C:\CDI32\snlc2579.stp
BoardDegC    29.5
ArrayDegC    27.2526
TECA   0
ExtV         -17.2354
DacOffset    3546
IntTime      0.000819
Processing   none
CalUnits     A/D Counts (Subtract Background)
TrigMode     TM_SynchRead
SampleAvg    1
Scans Averaged     1
WaveUnits    nm
WaveStart    432.115
WaveEnd      959.617
WaveStep     2.06055
**HeaderEnd**
600    -7474.793
600.5 -7292.662
601    -7118.225
601.5 -6948.744
602    -6823.884
```

Figure 9.1.

9. Open an ASCII Trace File

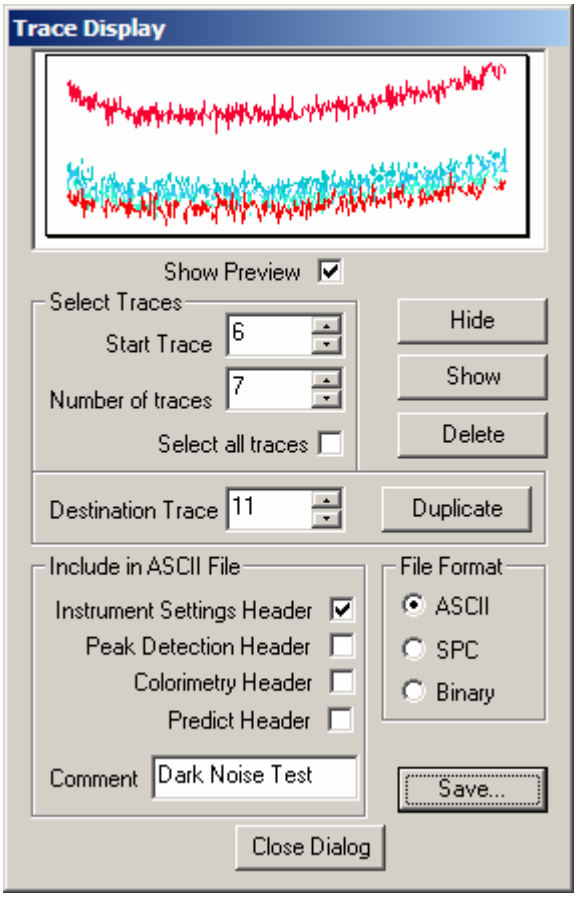
Access the menu bar and click **File | Open Trace…** or tool bar  to open a trace. When the **Open Trace** dialog box comes up, select the desired trace file that you want to open and click **Open**.

10. Open a Binary Trace File

A grouping of trace files with extension ".g00" is a **Binary** file. To open a **Binary** trace file, access the menu bar **File | Open Trace…** or  . When the Open Trace dialog box comes up, click on the arrow-down on the right of the **Files of Type** text box and scroll down and select the "*.g*" entry. **Binary** trace files whose names match that pattern, such as "test.g01" or "samples.g0003" will be listed in the open trace file dialog, as the "*" serves as a wildcard for any number of characters. Select the Binary trace file that you would like to open and click **Open**.

11. File | Save Trace….

To save a trace, access the menu bar and click on **File | Save Trace…** or click on the  icon on the tool bar. The Trace Display dialog box comes up.



11.1. Show Preview

This small window displays a preview graph consisting of all the traces selected by the trace selection controls described in the next section.

11.2. Select Traces

11.2.1. Start Trace

Selects the first trace in the range to be selected. Click the small up or down arrow on the right of the text box to adjust which trace to start at.

11.2.2. Number of Traces

Select the number of traces to be acted upon at by using the up or down arrows on right of the text box. For example, to save traces 2 through 5, one would select a start **Start Trace** value of 2, and set this parameter to 4 traces, selecting the **Binary** (.g00) File Format and finally clicking the S**ave…** button.

Note: If only one trace is present, then the options **Start Trace** and **Number of traces** will be disabled grayed out (disabled).

11.2.3. Select all traces

This will select all the traces on the graph window.

11.2.4. Hide, Show, and Delete Buttons

The **Hide** button hides the selected traces on the graph window. The **Show** button makes them visible again. The **Delete** button permanently erases the selected traces.

Note: Trace 0, the blue-green trace first seen at startup, cannot be deleted.

11.2.5. Destination Trace and the Duplicate Button

Select the desired trace number in the **Destination Trace** text box, then click on the **Duplicate** button. An identical trace will be copied and placed into the specified slot, potentially overwriting an existing trace. By default, the duplication is configured to produce a new trace that will not overwrite any existing ones. For example, if the

highest numbered trace is trace 8 (there are 9 traces), set the destination trace to 9 to avoid overwriting any other traces.

11.3. Save…

There are available three file formats in which Spec32 can save a trace.

11.3.1. ASCII

Selecting this radio button and click **Save…** button will save the trace in ASCII file, see **Figure 9.1,** with file extension DAT. All selected traces will be saved as individual files.

11.3.2. SPC

Selecting this radio button and clicking **Save…** will save the trace in the SPC file format described in the previous section. All selected traces will be saved as individual files.

11.3.3. Binary (*.g00) files.

Selecting this radio button and clicking **Save…** will save the selected traces all together as one file with the extension "g00". A trace saved in this binary format cannot be edited with a text editor. The file size (per trace) for this format is much smaller than one saved in ASCII.

11.4. Include in ASCII File

These check boxes enable the outputting of various informative headers along with the spectral data for the trace. However, they only work with the ASCII (*.DAT) file format.

11.4.1. Instrument Settings Header

Outputs a header with basic information about the unit and the unit's configuration, as well as the computer used to sample the data. This information updates automatically.

11.4.2. Peak Detection Header

The most recently calculated peak detection settings will be saved in a header when a trace file is saved. Enabling "Online Peak Detection" in the **Peak Detection** dialog box will ensure that each time a sample is acquired, the peak detection information will be recalculated. Also, since peak detection cannot be made "Online" for traces other than Trace 0, take care to calculate the peak detection information manually before saving traces other than Trace 0.

11.4.3. Colorimetry Header

If Colorimetry data has been calculated, this will cause those results to be output in a header when saving traces. Please ensure that "Online Colorimetry" is enabled so that the calculations are concurrent with the trace saved.

11.4.4. Predict Header

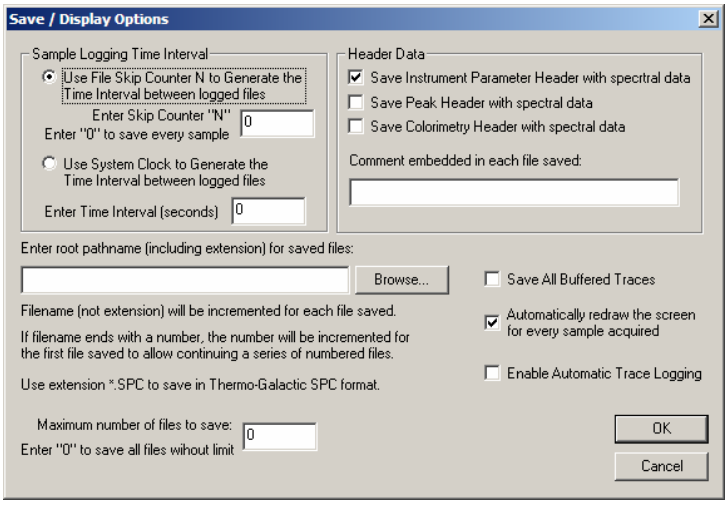
If Grams IQ Prediction is installed and enabled (see Appendix B of this manual), having this setting checked will cause the prediction results to be saved in the trace file. Having "Online Prediction" enabled helps ensure that the prediction results are concurrent with the trace being saved.

11.4.5. Comment

Text input box for a user defined comment that will be outputted along with the **Instrument Settings Header**, if enabled.

12. File | Trace logging…

Trace logging saves traces automatically during acquisition. This is useful when you are taking samples and want all traces saved automatically. Click on **Trace Logging** from the file menu, and a window comes up, **Figure 11.1.**



Select the check box "**Automatically save every "nth" file to the root pathname".** Type in the number in the **Skip Counter** text box to skip or leave it at the default value of "0" to save every sample.

Enter the complete pathname to destination directory to save the traces to, or click on the **Browse…** button and select the destination folder in the file dialog window. The filename will be incremented for each file saved. If the filename ends with a number, that number will be incremented for the first file saved.

Enter the maximum number of files to be saved, or enter "0" to save all files without limit.

Select the header data to be saved with the spectral data, if any.

Check the box "**Automatically redraw the screen for every sample acquired"** to redraw the spectra on the screen (normal operation).

If the check box "**Save All Buffered Traces**" is selected, then all the traces will be downloaded from the buffer and saved to individual files (only when in Fill Buffer mode) on every update.

Finally, and most importantly, remember to select "**Enable Automatic Trace Logging**" to turn on the data logging.

Chapter 5
Using the Setup Command Menu

Select **Setup** from the menu to access all the setup commands that let you change the setting of how your spectrometer takes samples and to change the Hardware Setting of the spectrometer. You can use these setup commands to change the colors a trace, label a trace or delete a trace.

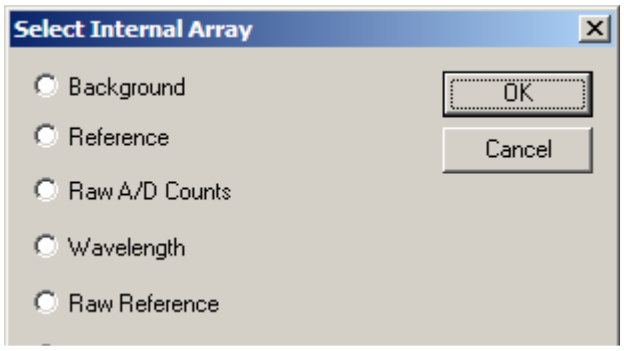
1. **Setup | Trace Display…**

   Trace Display is the same as **File | Save Trace…** It is duplicated here under the Setup menu with the other graph and trace display commands for convenience. Please refer to **Section 10.1 File | Save Trace…** for more information of how to use **Trace Display** dialog box.

2. **Trace Header Display popup menu**

   It is possible to view header information for a trace which has been loaded using **File | Open Trace** by right clicking one of its data points on the graph display. A popup menu will appear with an option called **Show (Retrieved) Trace Data**. That will use the same dialog box as this menu command, but will populate it with header information found in the trace file (if any). It also displays the trace number in the window title bar.

3. **Setup | Show Internal Array**



   This dialog can display many different internal data arrays that may be of interest. For example, if one has stored a reference with the Acquire Reference command, the user can use this dialog to load the Raw Reference as a trace on the graph window to examine it. Some of the internal arrays have limited uses to an end user, besides diagnostics information. However, the following arrays may be very useful for a user:

   - Background
   - Reference
   - Raw A/D Counts

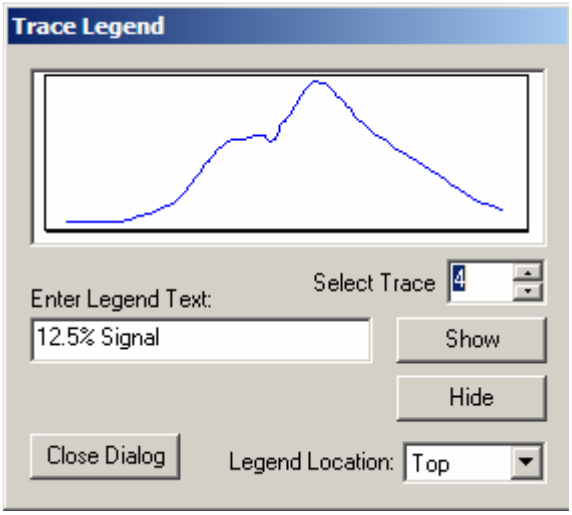
- Wavelength
- Raw Reference (Reference without amplitude linearization or background subtracted)
- Cal Source (AutoCal output)

4. Setup | Unhide Traces

This command simply makes visible any traces that have been hidden by the Trace Display dialog mentioned in **Section 1**.

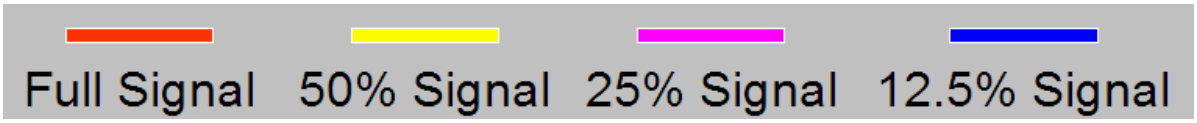
5. Setup | Trace Legend…

5.1. The Trace Legend Dialog box



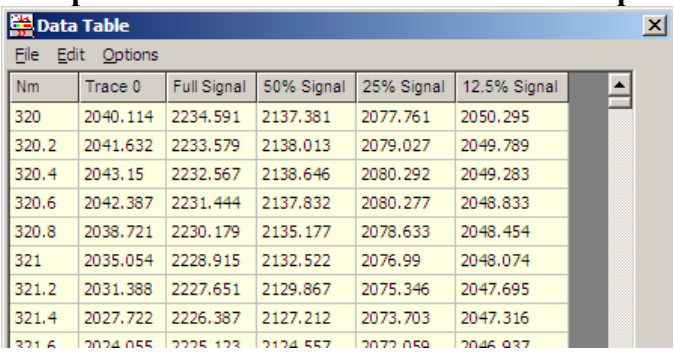
The **Trace Legend** dialog makes it possible to label one or more traces. Select a trace number from the **Select Trace** text box. Enter the name for that in the **Enter Legend Text** box. Click on **Show** button and it will display the legend text for the selected trace on the screen, or click on **Hide** button to hide the legend for that particular trace. The **Legend Location** drop down menu can configure the position of the legend markers relative to the main graph window.

5.2. Example Legend Markers



6. Setup | Trace Data Table

6.1. Sample Trace Data From the Previous example



Nm	Trace 0	Full Signal	50% Signal	25% Signal	12.5% Signal
320	2040.114	2234.591	2137.381	2077.761	2050.295
320.2	2041.632	2233.579	2138.013	2079.027	2049.789
320.4	2043.15	2232.567	2138.646	2080.292	2049.283
320.6	2042.387	2231.444	2137.832	2080.277	2048.833
320.8	2038.721	2230.179	2135.177	2078.633	2048.454
321	2035.054	2228.915	2132.522	2076.99	2048.074
321.2	2031.388	2227.651	2129.867	2075.346	2047.695
321.4	2027.722	2226.387	2127.212	2073.703	2047.316

6.2. Details

Click on **Setup | Trace Data Table** to open a small window that displays the data of the traces that are currently in memory. This is useful for querying the exact numerical values of the traces. Tables consisting of at least two columns are shown. The first column is labeled "Nm", and the second column is labeled with the trace legend text if you have previously given one; otherwise, the default trace with label "Trace 0" will be displayed. The data in this grid control can be copied and pasted into your favorite spreadsheet program.

7. Setup | Delete All Traces

Deletes all traces that are currently stored in the computer's memory, Trace 0 being the exception. To delete a single trace, use the **Trace Display** dialog and select the trace to delete, and click on the **Delete** button.

Warning: There is no "undo" feature for deleting traces. Once deleted, they cannot be recovered.

8. Setup | Integration Time…

Integration time is the electronically configured exposure time of the array. Signal level is typically proportional to integration time. The longer the integration time is, the higher the signal is shown on the screen (if in Raw A/D Counts Mode). This dialog box allows the user to configure the integration time. Enter the integration time in second(s) in the box and click **OK**. Entering 0 and clicking **OK** will set to the lowest exposure time you can set. If the spectrometer is saturating high at the minimum integration time, it may be due to the intensity of the light source. In that situation, it would be necessary to reduce the brightness of the light source by using one or more neutral density filters.

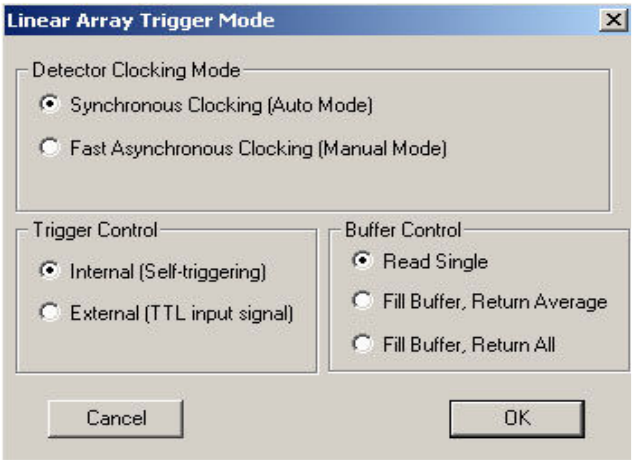
Tip It is convenient to use the **Auto Configure** to determine an **Integration Time** that achieves a good level of signal without saturating, which is 50,000 counts or so. After the command is run

the unit should be running at an integration time that achieves this signal. In the absence of a light source the command will likely fail, however.

9. Setup | Trigger Mode…

9.1. Linear Array Trigger Mode Dialog

The **Linear Array Trigger Mode** dialog box appears, as depicted in the image below**.**



9.1.1. Detector Clocking Mode

9.1.1.1. Synchronous Clocking (Auto Mode)

Synchronous clocking is a sampling rate and controlled by hardware built in the spectrometer. This sampling rate is constant. This mode is good for fast repetitive sampling with short integration time. By default, this mode is enabled.

9.1.1.2. Fast Asynchronous Clocking (Manual Mode)

Asynchronous Clocking is a manual sampling rate that's controlled by the software or external signal. That means the spectrometer doesn't start taking samples until the **Scan Single** button is pressed or triggered by an external signal over a wire. This mode is good for taking samples by using external triggers, on-line processing or where precise timing is critical.

9.1.2. Trigger Control

9.1.2.1. Internal (Self-trigger)

This is the software-controlled mode. No external signal is required.

9.1.2.2. External (TLL Signal)

In this mode, the trigger signals come from an external device.

In this mode, the detector is held in reset until the external trigger is received. Then the exposure starts when the trigger is received.

The advantage of this mode is fast triggering on events, with all samples stored in the FIFO. The sample timing is synchronized to an external device. Thus, the sampling is more concurrent with outside processes.

9.1.3. Buffer Control

9.1.3.1. Read Single

When this option is selected the data is sent to the screen after each sample is taken. This provides immediate visual feedback while making integration time adjustments. This mode is almost as fast as the Fill Buffer mode for integration times greater than 110-mS.

9.1.3.2. Fill Buffer, Return Average

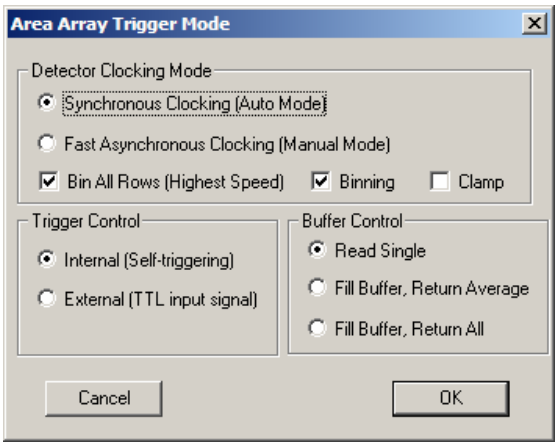
When this option is selected it causes the on-board FIFO memory to be filled before any spectral data is updated to the screen. This can be used for increasing the acquisition rate for integration times shorter that 110-mS. **Fill Buffer** mode is preferred whenever update time permits. This mode is not compatible with **Asynchronous Clocking**.

9.1.3.3. Fill Buffer, Show All

Same as the previous mode, but displays each spectrum in the buffer as a unique trace on the screen.

9.2. Area Array Trigger Mode Dialog

When using a spectrometer that has an MPP (area array) detector, the following dialog will be displayed instead of the **Linear Array Trigger Mode Dialog**.



9.2.1. Detector Clocking Mode

The discussion about synchronous and asynchronous clocking from the Linear Array section above still applies.

Three additional settings are present that are unique to area arrays, however.

9.2.1.1. Binning

Binning causes an area array to behave similarly to a linear array, in that the number of pixels of data read out is the same as the number of columns as the area array. In essence, the rows of each column are averaged together to form a single column value. However, a small number of rows on area arrays are non functioning (dark) by design and do not contribute useful information to the binning.

Binning provides a speed advantage over not binning, as many rows can be averaged together and outputted simultaneously. Otherwise, each rows would be read out, which is expensive in terms of time. Under normal circumstances, this mode will filter out inoperative rows of the area array, causing some delay in acquiring the data.

9.2.1.2. Bin All Rows

This Bin All Rows triggering mode is the fastest MPP sampling mode because it includes the dark rows in the signal. It is approximately twice as fast as just using **Binning** by itself. The Binning checkbox must be checked as a prerequisite for using this mode.

9.2.1.3. Clamp

When enabled or disabled, the clamp may reduce the sampling noise.

9.2.2. Trigger Control

Consult the Linear Array sections on triggering mechanisms as the details are the same.

9.2.3. Buffer Control

Consult the Linear Array section on using the buffer and single reads as the details are the same.

10. Setup | Use Ext. Trigger Sensor

This command enables a "hybrid" trigger mode to utilize the synchronous clocking mode with an external "start" signal. This allows more flexibility in sample parameters, such as averaging and fill buffer modes, and utilizes the most stable operating mode of the detector (synchronous clocking mode, internal trigger). The external trigger sensor is sampled by software, and when the trigger signal is present the software initiates the capture of the spectral data. This mode is especially useful for sampling kinetic data.

11. Setup | Free Running Manual Mode

This mode of operation is for low-latency sampling using the asynchronous clocking mentioned in the **Trigger Mode** section. The software will wait for a sample to complete, then immediately trigger the next sample after it reads the most recent acquisition. Thus, the next sample will be in the process of being acquired while Spec32 does other processing and then later asks to read it back from the spectrometer.

12. Setup | Set Buffer Size

Spectrometers using USB 2.0 HiSpeed firmware can the buffer size arbitrarily small (1 sample) or large (up to 2048 samples.) All previous firmware utilized a hardware buffer, called a FIFO. Thus, the buffer size varied from unit to unit. The HiSpeed firmware utilizes a fast software buffer that constantly reads the spectrometer output in the background until the buffer is full. One way to verify that the HiSpeed firmware is running is to invoke this menu command, change the buffer size to something other than what it previously was, and

then click the menu command again. If it changed, the HiSpeed firmware is active. See the section covering HiSpeed firmware for more details.

13. Setup | Amplitude Calibration

The amplitude calibration dialog box contains all the controls for spectroscopic calculations. Although the radio buttons for selecting "Amplitude Calibration Units" are also represented in the **Amplitude Calibration** list box of the control bar, the options described below must be selected in this window.

13.1. Select Reference

These radio buttons configure where the reference spectrum is obtained from.

13.1.1. Current Internal Reference

This selection causes only the sampled and stored reference signal to be used in the calculation of spectroscopic units. That is, references stored using the reference toolbar buttons and their corresponding menu commands.

13.1.2. Binary Reference File Data

The selection causes the binary reference file entered in the provided edit control to be loaded from disk into the internal Reference table. The existing internal Reference table is replaced with the selection. The binary reference file must be created by sampling a reference using the same spectrometer and then saving the setup file to create the *.REF file.

13.2. Calibrate to External File Data

The complete filename for the file containing the calibration data may be entered directly into the edit control provided, or the "File…" button may be pressed to browse for the file. Whenever the "Calibrate to External File Data" option is selected for Calibration Units using either the control bar Amplitude Calibration list box or the Amplitude Calibration dialog box. The file data specified in the edit control will be used in the calculation of spectroscopic units. Further info on using this compensation mode is available in the Appendix.

13.3. Convert All Traces

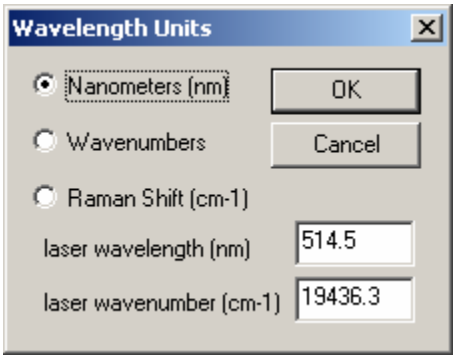
When this checkbox is checked, all the traces in memory will have the changed (if any) settings applied to them. There may be times where it is not desirable to leave this checked. For example, if one were to load a previous trace that was created in the Percent Transmittance compensation mode, but at runtime was loading it while in the Raw A/D counts compensation mode, he would likely not wish for the previous trace to be treated as raw counts during a switch to some other compensation mode.

14. Setup | Wavelength Interpolation

Wavelength interpolation is the linear interpolation of the data points to provide evenly spaced data in the wavelength axis. Most data processing algorithms require input data to be provided as evenly spaced points. The interpolation algorithm is simply a linear interpolation that connects adjacent data points together that satisfies the step size specified. This is a reversible operation in that the internal uninterpolated data is still available after applying interpolation.

To use wavelength interpolation, select **Setup | Wavelength Interpolation**. Enter the spectral range and resolution required. This can provide the opportunity to "ignore" certain wavelength ranges that are not of interest in a sample. Check the box " **Enable On – Wavelength Interpolation**" to interpolate the spectrum in real time; that is, after each acquisition the result will be interpolated before being displayed. The box "**Apply to all traces**" is optional – it will interpolate any other traces visible on the graph after hitting **OK** to close the dialog box. If not checked, only Trace 0 will be linearly interpolated on closing the dialog box.

15. Setup | Wavelength Units



The Wavelength Units dialog box

The horizontal axis of the graph window can be expressed in multiple types of units.

15.1. Nanometers

The typical unit used is the nanometer, corresponding to the wavelengths of light being queried by the spectrometer's detector array.

15.2. Wavenumbers

For some applications which typically involve Near Infrared (NIR), it is considered useful to express each wavelength as a wavenumber. The conversion between wavelength expressed in nanometers and wavenumber expressed in inverse centimeters is easily remembered as the following formulas:

- $\lambda = 10{,}000{,}000 / \nu$
- $\nu = 10{,}000{,}000 / \lambda$

Where λ represents wavelength (nm) and ν represents wavenumber (cm^{-1}).

15.3. Raman Shift

Raman spectroscopy often requires the use of a wavenumber offset that corresponds to the wavelength of the monochromatic light source used to exite the molecules in a sample. CDI spectrometers employ a laser as the excitation light source in Raman spectrometers. The two edit boxes can be used to enter the wavelength (or wavenumber) of the monochromatic source. Of course, this setting has no effect over the physical wavelength of the source, it just adjusts the expression of the X axis.

The X units in this mode are simply the wavenumber axis but all the coordinates will have the wavenumber of the monochromatic source subtracted.

16. Setup | Graph Settings…

Graph settings are customization options where many settings for the look and feel of the CDI Spec32 graph window can be changed. Examples of such settings are the font size, the background color, or turning grid lines on and off… See the Appendix for a detailed description of the options available.

17. Data Cursor On

Toggles a cursor the shows a graph-wide cross hair that can be positioned on a part of the graph. In the upper left hand corner of the graph, a pair of coordinates (X, Y) will be shown giving exact position for that point on the graph. As new data is periodically acquired this cursor will also update its position and coordinates.

18. Hardware Setting…

18.1. Hardware Setting | Temperature Setpoint…

This command allows one to configure the temperature set point for spectrometers with a built-in array cooler. The temperature setting is in degrees Celsius. To set the temperature, enter the set point in the text box and click on **Cooler** on check box to enable the cooler if the box is not already checked. Click on **OK** to finish.

Note: The lower the temperature set point relative to the ambient temperature, the more current will be drawn to operate the cooler. Setting the temperature too low will cause the spectrometer to lose stability.

18.2. Set DAC BaseLine

Use this command when you run the spectrometer, and it is saturated low. What the software does is to check for saturation levels, and set the analog baseline to maximize the usable A/D converter range by adding 2,000 counts to the baseline. Make sure to turn off the light source or shutter the light source before running this command (if automatic shuttering is not available.)

18.3. Change Analog Offset Counts

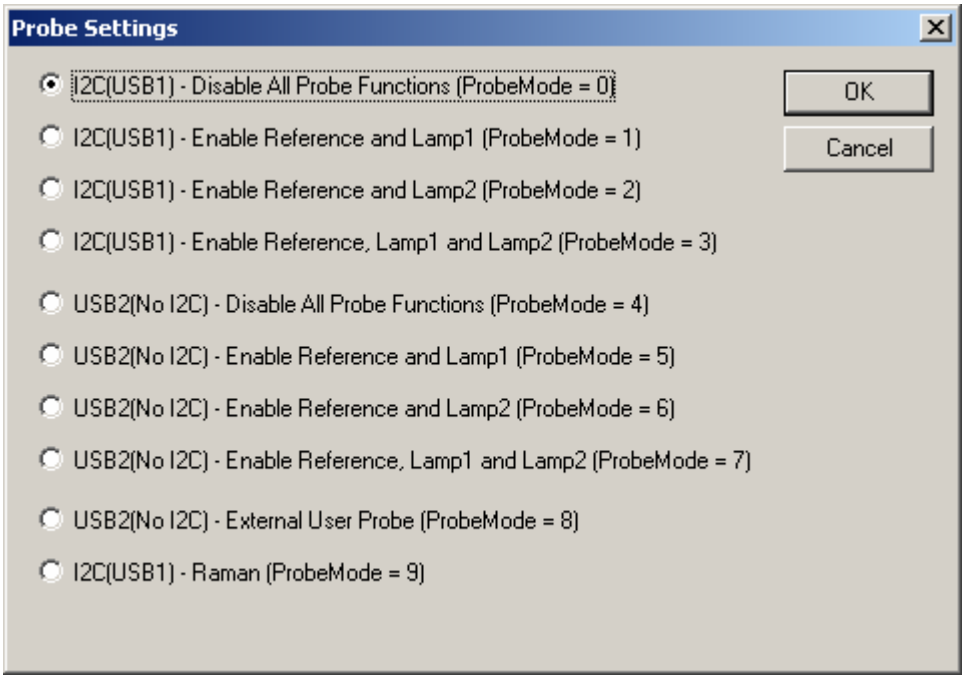
Sometimes the 2,000 offset count default is unsuitable for an application, as it could cause saturation (65,000 counts or higher at any point) in some situations. Or perhaps the output of the spectrometer is such that it saturates low (0 counts at any point). If the output if the graph is just slightly too high or slightly too low, this command can be used to vary the offset. The number of counts presented in this dialog box does not correspond exactly to the output offset, so it may take some repeated adjustments to come to a satisfactory offset.

18.4. NIR High Gain Mode

This option will cause NIR spectrometers to run in high sensitivity mode. It will make the spectrometer take samples 16 or 21 times faster than in low sensitivity mode. On the downside, the amplitude response can become much more non-linear. By default, high gain mode is turned off.

Note: Only use this mode when high speed is essential to the acquisition process.

18.5. Probe Settings



This dialog allows the use of an external or attached probe. Most units do not have such hardware, but for those that do, this controls which outputs are used and how they are used. I2C (Inter-integrated circuit) interface probes are used with spectrometers prior to USB 2.0. Probe modes 0-3 and 9 should be used with those, and probe modes 4-7 should be used with USB 2.0 units. Probe mode 8 is reserved for special applications and should not be used.

18.6. Probe Mode

Same as the command above but simply provides a dialog box to enter the probe mode number, without any other indications of what the probe mode does.

18.7. Probe Reference

Toggles the probe reference paddle state, if present. When checked, the reference paddle will be in the way of the light path, reflecting the lamp output back into the probe head. This would be used when taking a background or a reference on a probe, the background being taken with the probe's light source turned off.

18.8. Probe Lamp

All probe assemblies come with one or two tungsten light source lamps. This command toggles Probe Lamp 1 on and off. Please note that some spectrometers only contain a light marked as Probe Lamp2; sidecar lamp systems are an example of this.

18.9. Probe Lamp2

Like the previous command, toggles the on / off state of the second Probe Lamp, if present.

18.10. Bg Delay

Configures the wait time (in milliseconds) between the time when the lamp is turned off and when background is sampled during automatic background and reference acquisitions.

18.11. Ref Delay

Similar to the above setting (**Bg Delay**), this controls the wait time (in milliseconds) between the time when the lamp is turned on and when the reference is sampled during automatic background and reference acquisitions.

18.12. AutoCal Calibration

Performs an AutoCal calibration that calculates the change in the wavelength calibration from the factory calibration. Once the shift has been determined, it will be applied. The amount of time it takes to complete will vary based on the **AutoCal Settings** below.

18.13. AutoCal Source On

Units that have AutoCal enabled come with an elemental light source, which is typically Mercury-Argon [HgAr] or Neon [Ne]. This setting toggles the state of that light source as being on or off. During an AutoCal acquisition, particularly with probes, this state may be automatically controlled, however.

18.14. AutoCal Settings

Specifies the initial integration time and warmup time for taking AutoCal samples at. This integration time may change during the AutoCal process so that spectral lines from the lamp can be more easily seen.

18.15. Initialize AutoCal

Initializes the state of the calibration source and the reference paddle, and performs the first calculations needed to do subsequent AutoCal measurements. Note: this is only used for the optional "Always On" autocal configuration, which requires a special probe.

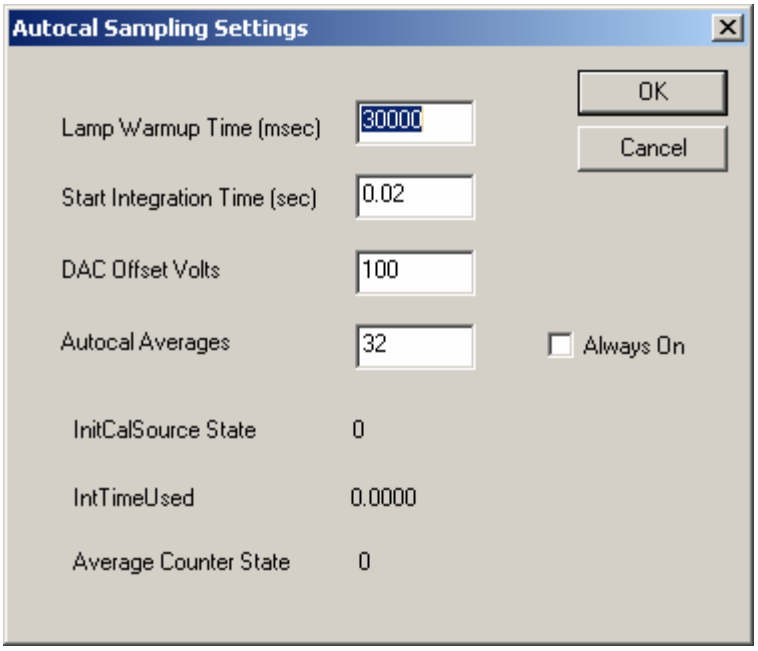
18.16. Sample AutoCal Background

As the name implies, does the processing necessary to store a background for use with an AutoCal measurement. Normally the background acquisition is handled as part of each autocal operation, but this option is available for use with the optional "Always On" autocal configuration. Note: this is only used for the optional "Always On" autocal configuration, which requires a special probe.

18.17. Sample Single AutoCal Spectrum

Like the last command, this is for piecewise acquisition of the AutoCal main spectrum. That is, it is the spectrum that will be used to perform the calibration adjustment. Note: this is only used for the optional "Always On" autocal configuration, which requires a special probe.

18.18. Set AutoCal Averages



As the picture depicts, allows the user to set more than just the averages for AutoCal. The warmup time and integration time, as well as the DAC offset for the AutoCal sampling can be configured here. The number of samples that are averaged together is specified in the fourth edit box. The "AlwaysOn" checkbox, if checked, will cause the AutoCal light source to always be turned on during spectrometer operation. This can help with the stability of the samples.

The text labels below simply give feedback on the current state of AutoCal. "IntTimeUsed" corresponds to the discretized integration time read back from the spectrometer, as it tends to vary from the inputted integration time.

18.19. Get AutoCal Settings

This brings up a much more concise dialog with the same information as the previous dialog, but the information is entirely read only.

18.20. Compute AutoCal Adjustment

Allows the autocal to be computed from stored data, i.e. a trace of the AutoCal source.

18.21. Shift Wavelength Calibration

Allows the adjustment of the wavelength calibration scale with a fixed offset.

18.22. Remove Pixel

Removes a pixel from being displayed on the graph, and from the internal calibration. It is not recommended to use this feature unless instructed to do so by CDI staff during a tech support session. Some detector arrays may have a bad (unstable) pixel which needs to be removed.

18.23. Fan Switch Toti

Sets the T_{OTI} (Overtemperature Indicator) temperature for the fan system. The value is expressed as a signed integer that represents a degree value in the Celsius scale. The range is from -127 to 127 degrees. If the temperature of the unit exceeds this value, the fan will be turned on in order to cool the unit. It is not recommended to change this value unless a very specific set point is needed. Normally the fan is controlled by setting the T_{OTI} to the lowest possible temperature to turn on the fan, and the highest possible temperature to turn on the fan. If the fan is switching on and off periodically, it can affect the stability of the spectrometer due to changes in the amperage required to run the spectrometer varying.

18.24. Fan Switch Thyst

Sets the T_{HYST} (Hysteresis) temperature for the fan system. The value is expressed as a signed integer ranging from -127 to 127, and like the T_{OTI} setting above, it is expressed in degrees Celsius. If the temperature of the unit falls below this value, the fan will be shut off as the unit no longer requires cooling. See the above section on T_{OTI} for cautions against changing this value.

Chapter 6
Using the Process Command Menu

1. Process | Derivative…

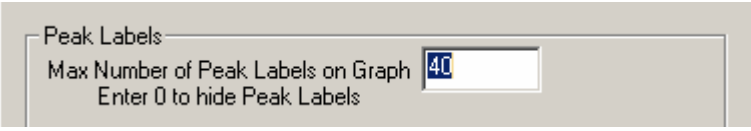
"Derivative" corresponds to the Savitsky-Golay smoothing algorithm. To use this command, click on **Process** from the menu bar and select **Derivative** and a dialog box comes up. Enter the number of points in the text box. Click on the arrow down to the right side of the **Savitsky-Golay Method** and select the method that you would like to use. Click on **OK** button to proceed. It will take a few seconds to process this command. To undo the Savitsky-Golay processing, do the following:

2. Revert (No Processing)

This will do exactly what it says. This command will undo the **Derivative** process. Click on **Process** and select **Revert** to proceed.

3. Peak Detection

Initiates an algorithm that takes the data of a particular trace on the screen (by default, Trace 0) and calculates the local maxima; that is, the highest local points of the data. There are many parameters that can be adjusted to change the peak detection method and filtering of the peaks once they are detected. A fresh installation of Spec32 resets this number to 0.



3.1. Peak Labels

The internal peak detection data is capable of storing 150 individual peaks.

3.2. Peak Label Text Size and the Select Color Button

Sets the font size of the peak labels. The **Select Color** button brings up a color picker dialog that sets the color of the peak labels.

3.3. Repositioning Peak Labels with the Mouse

This feature is not enabled at this time, but may be available at a later date.

3.4. Text Label Contents

- Wavelength, Amplitude – Displays the calculated X coordinate and Y coordinate of each peak.
- Wavelength (only) – Displays the calculated X coordinate of each peak.
- Wavelength, FWHM – Displays the calculated X coordinate and FWHM (Full Width at Half Maximum) of each peak.
- Wavelength, Area – Displays the calculated X coordinate and the accumulated area underneath the peak. Area is calculated from the left base coordinate to the right base coordinate.

3.5. Detection Method

Sets the detection method for calculating the local maxima. The available methods are:

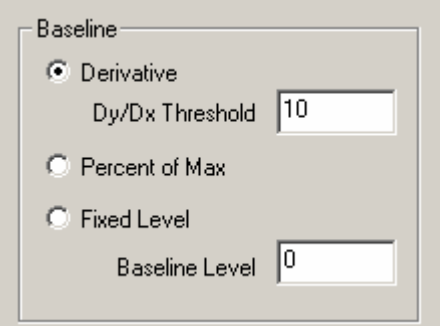
- Peak Wavelength – Simply outputs the maximum value that occurs between the base coordinates. The wavelength is the data point at which this occurs.
- FWHM Center Wavelength – The peak wavelength (X coordinate) is calculated from interpolated data by using the amplitude at the Peak Wavelength value above, and determining the locations in between the base coordinates where half the Peak Wavelength amplitude occurs. The midpoint between those two locations is where the FWHM Center Wavelength is calculated. The wavelength and amplitude is calculated as the interpolation between that data point and the next adjacent data point. The resultant values are almost always not part of the graph itself.
- Centroid – Performs a COG (Center of Gravity) calculation to determine the wavelength and amplitude of each peak.

3.6. Peak Table Display Setting

Wavelength	Amplitude	FWHM	Area
693.914	43047.3	77.5048	2.59889e+006
673.369	41941.8	68.4171	2.11014e+006
525.76	26259.3	96.3293	1.87798e+006

If this edit box is set to a nonzero value, a peak data table containing no more than the specified number of peaks will be displayed along with the graph. The data table (a sample is depicted above) contains information most commonly needed for peak detection applications.

3.7. Baseline



- **Derivative** – The bounding (baseline) coordinates for the peak detection are determined using the discrete derivative at each point of the graph. Each left base coordinate exists at the point where the slope of the graph reaches at least the value specified by **Dy/Dx Threshold**. The right base coordinate exists where the derivative reaches the negative of **Dy/Dx Threshold**.
- **Percent of Max** – First, the maximum value on the whole trace is determined. Then, this percentage (specified by **Baseline Level**)
- **Fixed Level** -

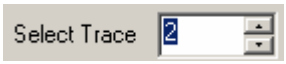
3.8. Peak Threshold

Once peak detection has occurred, this value sets a minimum allowable amplitude for a peak to be included in the final set. This is used in practice to filter out peaks with lower amplitudes that may be more subject to noise. Set this to a sufficiently low value if this sort of filtering is not desired.

3.9. Online Peak Detection

If checked, peaks will be recalculated each time Trace 0 on the graph is updated. That is, every time a new spectrum is obtained.

3.10. Select Trace



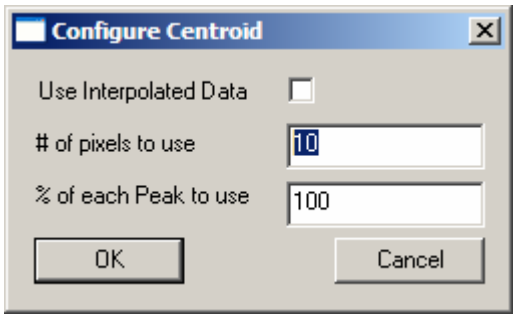
The trace that will be used to calculate the peak data. Note that online peak detection will not work with traces other than Trace 0.

4. View All Peak Data

Peak Number	FWHM Ctr Wav	Centroid Wav	Peak Wav
0	377.9553	378.0328	377.9553
1	380.1948	380.2092	380.1948
2	383.5377	383.5421	383.5377
3	388.0166	387.8553	388.0166
4	525.7597	517.5136	525.7597

Displays the wavelength (X coordinate) components for all of the internal peak data. Each peak detection method is represented. Useful for cross comparisons between the detection methods.

5. Centroid Parameters…



- **Use Interpolated Data** – Specifies whether the centroid peak detection method will use linearly interpolated data.
- **Number of pixels to use** – If interpolated data is not being used, this parameter can be used as a limiting factor to prevent the use of asymmetric peak data. This

parameter has no effect if **Use Interpolated Data** is enabled. The pixels used are centered around the highest point of the peak. For example, if 5 pixels are used, the pixel with the highest point will be used, as well as the two pixels to the left of the maximum and the two pixels to the right of the maximum.

- **Percentage of each Peak to use** – If not all of the peak is desired for use in calculating the centroid, a percentage can be specified to discard that data. Typically the reason for this is to avoid calculations on asymmetric peaks.

6. CIE Colorimetry…

Brings up a dialog that can enable the display of CIE XYZ colorimetry calculations and parameters. Either the CIE 1931 2° observer the CIE 1964 10° observer can be used. Can enable online colorimetry calculation which is useful for monitoring purposes and for trace logging. Please call CDI for any questions on how to use Colorimetry features.

7. L*a*b Colorimetry…

Brings up a dialog that can enable the display of CIELAB (L*a*b*) colorimetry calculations and parameters. Much like the previous section, this is a specialized feature and questions should be forwarded to CDI. An sample display from the colorimetry data table in Spec32 is depicted to the right.

8. Color Rendering Index

Brings up a dialog that specifies Color Rendering Index (CRI) settings and outputs in the colorimetry table. CRI is a method of determining how well the sampling light source induces color reflections in objects with respect to a perfect light source (black body radiation with a given temperature).

9. PLS Predict

Opens a dialog that handles PLS IQ Predict calculations. This is disabled unless a special additional installation has been done to enable IQ Prediction functionality. Consult the Appendix for information and instructions.

10. Verify Xe Lines

This outputs the accuracy of the wavelength calibration with respect to several prominent Xenon spectral lines, showing errors in both wavelength (nm) and pixel units. Must be run after peak detection has been done on a sampled Xenon line source.

11. Verify Hg Lines

Similar to the above **Veryify Xe Lines** feature, but for use with a Mercury Argon line source.

12. USP-1119 Test

This runs an automatic test designed for NIR reflectance probe systems to test compliance with the USP <1119> specification. In general, it tests:

- Wavelength Uncertainty (accuracy)
- Photometric Linearity
- Spectrophotometric Noise Flux

Appendix A
Calculating Spectroscopic Units

A spectroscopic unit is represented by the y-axis scale of the Graph and is shown in Counts, Percentage, Absorbance Units, Decibels, depending on what amplitude calibration is selected.

The calculation of spectroscopic units requires the calibration of each photo detector for wavelength, offset, and sensitivity. The offset and sensitivity must be calibrated for the measurement conditions and for the individual instrument in use to provide optimal performance. The values required for this calibration are discussed in this section.

1. Background

The Background is the zero light level, which consists of the array's thermal current and DC bias. The Background level is strongly dependent on the array's temperature and the array's integration time. Of course, the analog bias provided by the offset DAC must also be taken into account. The background data is sampled and stored in raw analog to digital converter counts, or A/D counts. To see how this reading is obtained during a test please review chapter 4 of the manual.

2. Reference

The Reference, or 100 percent light level, is sampled for the maximum light level to be measured. The Reference level is strongly dependent on the light source, the array integration time, and the optical response of the instrument including the input fiber and sample fixture. The Reference data is sampled and stored in raw A/D counts with the Background subtracted. The Reference minus the background is needed to calibrate the sensitivity of each photo detector.

When a Reference is sampled (absolute Reference), the Integration Time used to sample it is stored along with the Reference. If you want to change the Integration Time, a new Reference is calculated so that sensitivity remains the same. The software does this automatically so it is a seamless operation for the operator.

All spectroscopic units are computed with respect to the absolute Reference linearly scaled for changes in the integration time:

$R_N = (I_C / I_R) * R_A$

Where:
R_N = New Reference I_C = Current Integration Time
I_R = Reference Integration Time R_A = Absolute Reference

As the integration time is increased after the Reference is stored, the multiplier is proportionately decreased. The result is that the signal level in the spectroscopic unit does not change when the integration time is increased, although the signal raw A/D counts are increased. However, the signal to noise ratio may be increased with increased integration time.

3. Calibration Units

The Calibration Units are the units that the Y-axis of the graph is in with relation to the real world. For example it could be in Percentage of light, counts dB or Absorbance Units. These units are represented as a percentage of the Reference (100 percent).

For example, for Calibration Units in Percent, the Calibration Units will consist of the value of 100 percent for each photo detector. (Depending on which spectrometer you have, it could have anywhere from 256 to 1024 photo detectors in its array) The Calibration Units table may be any arbitrary mathematical quantity.

4. Spectroscopic Units

To compute Spectroscopic unit, the Sample to be measured must be sampled in A/D counts. The sample matrix is then converted to spectroscopic units.

$S = (1/r) * (S_C - B_C) * C$

Where:
S = Spectroscopic Units r = Reference Counts S_C = Sample Counts
B_C = Background Counts C =Calibration Units

4.1. Percent Transmittance (Reflectance)

Percent transmittance and reflectance are the simplest and most often used units. The calibration units are a constant 100 for each photodetector:

$\% = [(S_C - B_C) / r] * 100$

Where:
r = Reference Counts S_C = Sample Counts

B_C = Background Counts

4.2. Absorbance (Optical Density)

Absorbance units are the same as Optical Density, which is the log 10 (1/ Transmittance):

$AU = \log_{10} [r / (S_C - B_C)]$

Where:
r = Reference Counts S_C = Sample Counts
B_C = Background Counts AU = Absorbance Units

4.3. Calibration to a Blackbody Source

This calibration is used to compensate out the sensitivity variation due to the optical response and the photodetector response, effectively flattening the overall instrument response. The color temperature does not need to be exact to accomplish this objective. For this calibration, the Blackbody Calibration Units are relatively scaled intensity counts computed from the color temperature (°K) and the wavelength (λ) using Planck's blackbody equation:

$B_U = S_F * (C_1 / (\lambda / 1000)^{5.0}) / \exp (C_2/(\lambda * °K / 1000) - 1.0)$

Where:
B_U = Black Body Calibration Units S_F = Scale Factor (selected by the user)
C_1 = 37415.0 C_2 = 14387.9
Note: C_1 and C_2 have been re-scaled for calculation using λ in nanometers.

The output is then:
$RIC = [(S_C - B_C) / r] * B_U$

Where:
RIC = Relative Intensity Countsr = Reference Counts S_C = Sample Counts
B_C = Background Counts B_U = Black Body Calibration Units

4.4. External Amplitude Calibration File Format

The calibration data file must be an ASCII file, with two columns in the following format:
<Wavelength in nm><whitespace><amplitude><optional whitespace><newline chararacter>

Where whitespace includes all characters NOT in the string "0123456789+-eEgG".
An example of a single line of the file is like so:

400.0<tab>99.8<tab><newline>

Each line must be terminated with the new line character. This is the standard spreadsheet compatible ASCII formats. This file may be generated from Excel by saving a text format file. The wavelengths must be in ascending order. The data will automatically be linearly interpolated for use in the calibration.

The external calibration file can contain a header that describes

The units in this mode are derived in much the same way as **Percent Transmittance**, except instead of multiplying by 100 for each data point, we multiply by the corresponding value for each wavelength.

$U_E = [(S_C - B_C) / r] * M_E$

Where:
r = Reference Counts S_C = Sample Counts U_E = Final calibrated unit
B_C = Background Counts M_E = Multiplier for each wavelength in the cal file.

5. Sampling the Reference and Background

There are two commands available to sample and store the Reference and Background data: an automatic procedure and a manual procedure. These procedures are provided to ensure that the Reference and Background are stored in the proper units. It does not matter what Amplitude Calibration Units are selected, since these commands work on raw counts and may be performed at any time in any units to update the reference of background**.**

6. Automatic Procedure

Select the **Operate | Acquire Ref and BG** command.

This command will prompt the user to make the input dark (i.e. turn off the lamp or block the light path), then it will acquire and store the Background. Then it will inform the user that the Background has been stored. After the Background has been stored, another message box appears to prompt the user to connect the input to the reference (i.e. turn the lamp back on or unblock the light path), and the software will then acquire and store the reference. Finally, another message box appears to prompt the user to connect the signal to the input to be sampled.

The Background or Reference may be acquired separately with the same prompts and the same results using **Operate | Acquire BG** and **Operate | Acquire Ref**, respectively.

7. Manual Procedure

Connect the input to the spectrometer to the dark (0%) input. Disconnecting the fiber from the spectrometer input and covering the input connector may do this. However, it is preferable to shutter the light source. Do not turn off the light source, since it will usually need to stabilize for a few minutes after being turned on. Acquire a complete average, paying close attention to the status bar messages and watching the plot to determine stability. Then select **Operate | Store Reference / Background…** and check "Store Internal Background". The background has now been stored.

Connect the input to the spectrometer to the Reference (100%) input. Re-connect the fiber or open the shutter on the light source. Acquire a complete average paying close attention to the status bar messages and watching the plot to determine stability. Then select **Operate | Store Reference / Background…**, and check "Store Internal Reference". Make sure "Re-compute Amplitude Compensation" is checked upon storing the Reference. The Reference has now been stored.

The "Re-compute Amplitude Compensation" check box updates the Reference by subtracting the existing Background from the new Reference, and updates the Reference Integration Time. If the Reference is stored first, then checking "Re-compute Amplitude Compensation" when the new Background is stored will use both the new Reference and the new Background for subsequent calculation of spectroscopic units.

To update the Background without affecting the Reference, do not check the "Re-compute Amplitude Compensation" box when the Background is stored. This is the default behavior of the **Operate | Acquire BG** command.

It is often desirable to select "Internal Background" from the **Select Background** group in the **Setup | Amplitude Calibration** dialog box if you use the manual procedure. Using the **Zoom | Fit** (autoscale) command facilitates verifying the stability and noise on the Background and reference signals.

Appendix B
Using the Spec32 PLS Predict Feature

The PLS Predict feature allows an operator to directly predict the amount of a given constituent (such as moisture, API, excipients, fat, protein, etc…) present in a sample spectra. The predict feature currently displays up to ten simultaneous constituents in real-time. While this feature is not installed by default, this appendix describes the steps necessary to enable it.

First, one must have a PLS model ("___.cal" file) created using Thermo Electron Corporation's GRAMS/AI with PLSplus/IQ software application. Please see the GRAMS documentation for a full explanation on creating a PLS model.

1. Configuring Spec32 to perform predictions…

1.1. Install IQ Predict Standalone

To perform a prediction within Spec32, you must have Thermo Galactic IQ Predict Standalone properly installed on the computer running Spec32.

The Thermo Galactic IQ Predict Standalone application is not installed by default with the GRAMS standard installation. The installation files can be found on the Thermo Galactic GRAMS installation CD. (Typically: ("…\ DA\IQPR\ StandAlone\ setup.exe ")

1.2. Set the "PredictConfig" subkey…

The following entry must be present in the Windows Registry:

Location: [HKEY_CURRENT_USER\Software\CDI Spec32\Spec32\Settings]
Subkey: "PredictConfig"="C:\\CDI32\\CDI_PREDICT.IQS"

To add the entry, copy the "CDI_AddPredictKey.reg" file into the "C:\CDI32\…" directory and double click the file. A dialog will appear asking if you want to add the information to the registry. Click "Yes" to automatically update the registry. If your computer system will not allow external updates to the registry, you may manually add this key to the registry.

CAUTION: Manually changing the registry incorrectly can damage the operating system. If you are not comfortable making changes to the registry, please refer to a qualified individual for assistance.

1.3. Install CDI_PREDICT.IQS…

Simply copy the CDI_PREDICT.IQS file into the "C:\CDI32\" directory.

2. Establishing a PLS model…

The GRAMS/AI PLSplus/IQ add-on can be used to create a PLS model from "training" spectra saved in files. The following instructions describe a general approach to creating a model, though there are many variations depending on the application. Please consult the Thermo Galactic documentation for a full explanation of using PLSplus/IQ and building Data Sets.

2.1. Create SPC Files…

In general, you would start by using the Spectrometer system and Spec32 software application to obtain spectra of *calibration* samples with *known* concentrations of up to ten constituents. Save the spectra in standard SPC file format (header information is not required). Maintain a record of the constituents, and concentrations for each filename to be used while building the PLS model.

2.2. Create the PLS Model…

Use the PLSplus/IQ add-on within the GRAMS/AI application to build a PLS model. You will need to use the filenames and concentrations recorded earlier to create a new Data Set of constituents in PLSplus/IQ. The resulting PLS Model should be a "___.cal" file.

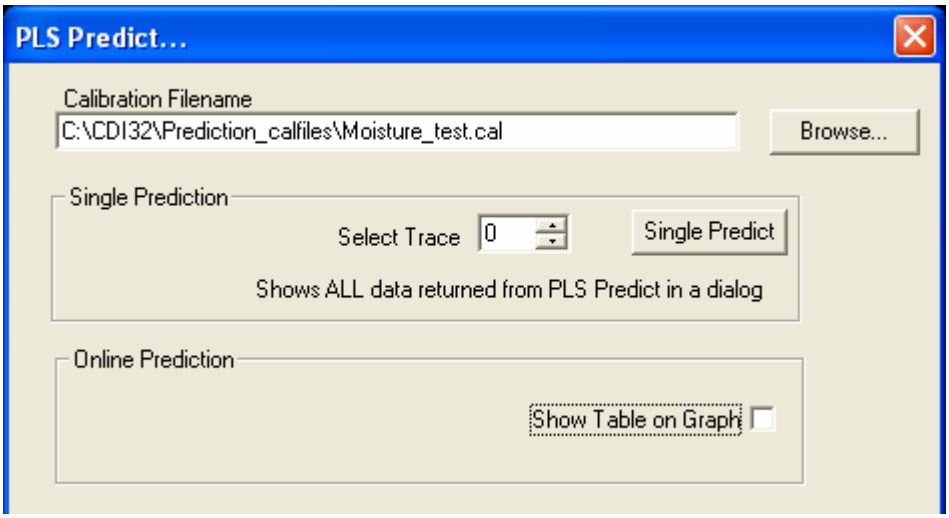
3. Performing a Prediction…

Spec32 can reference a completed PLS model to perform real-time predictions on sample spectra. The sample spectra (referred to below as the ***Trace***) should be similar to the spectra used to create the PLS Model, otherwise the IQ Predict function will convey "NO" match.

Note: If the *Trace* data falls outside of the model parameters, the IQ Predict function will fail and an error will be displayed. Check to be sure the spectrum units are compatible with the spectra used to create the PLS model. *Also, the sample Trace wavelength range must span at least as wide, or wider than the model range to avoid an error.*

3.1. Initialize Spec32 to use the PLS Model…

In the Spec32 menu click **Process | PLS Predict.** Browse to select the desired "____.cal" PLS model filename. Clicking OK will save the file choice, or you may select a prediction type (Single or Online).



3.2. Single Prediction

A single prediction can be performed on any *Trace*, but must be manually requested each time a prediction is desired. The first result window displays the report generated by the IQ Predict function. If the *Trace* does not fall outside the bounds of the PLS model, the second result window will show a grid display with all values reported from the IQ Predict function.

3.2.1 Execute a Single Prediction

After acquiring a *Trace* (or opening a saved Trace file), click **Process | PLS Predict**. Select the number of the desired *Trace* and click "Single Predict".

Note: If Single Predict is grayed out, uncheck "Show Table on Graph". Single Prediction and the Online Table cannot be shown at the same time.

3.3. Online Prediction

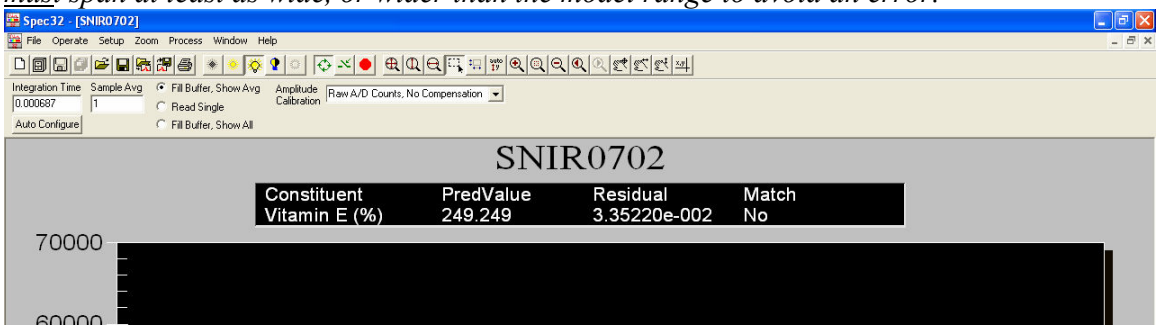
The online prediction will show a table above the graph with four columns that update in real-time each time *Trace0* is refreshed. Online prediction can only be performed on *Trace 0* (the active trace received from a spectrometer).

3.3.1 Execute an Online Prediction…

From the Spec32 menu, click **Process | PLS Predict**. Check the "Show Table on Graph" checkbox and click OK.

Each time the graph updates with a new spectrum in *Trace 0*, the table will update the values and constituents based on the PLS Model chosen.

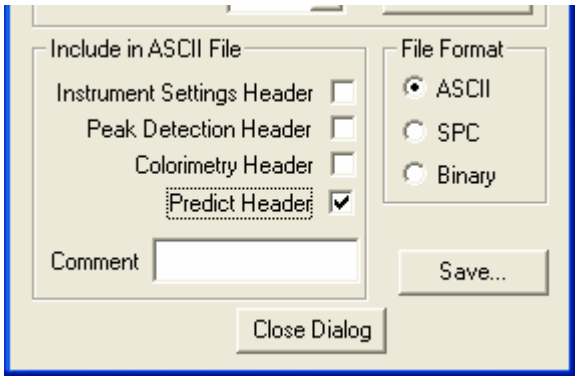
Note: If *Trace 0* falls outside of the PLS model parameters, an error will display for each constituent row. Check to be sure the spectrum units are compatible with the spectra used to create the PLS model. *Also, the sample Trace wavelength range must span at least as wide, or wider than the model range to avoid an error.*



3.4. Saving Prediction Results in a Trace File…

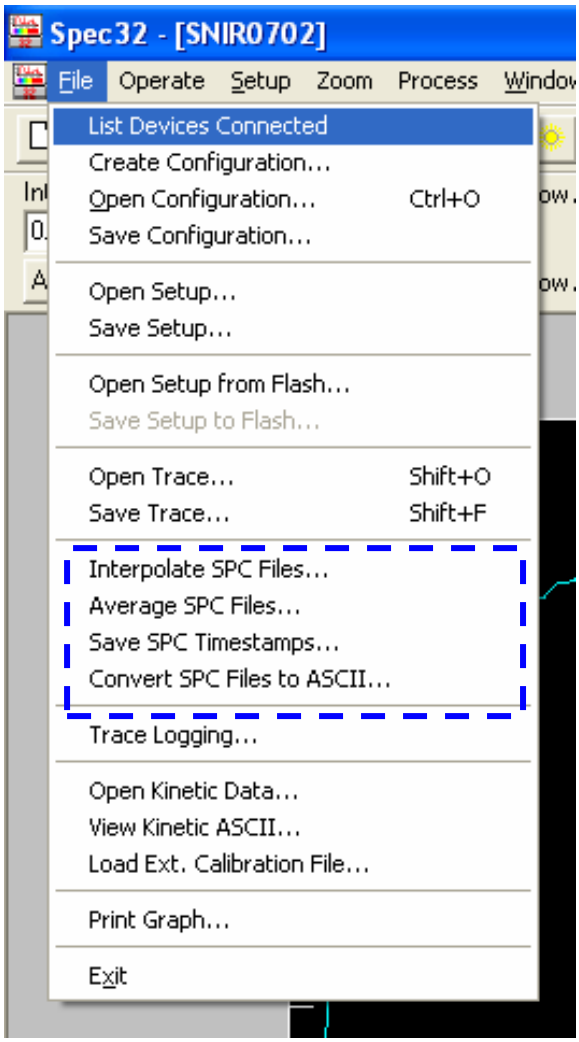
Predict results can be saved as Header information in any ASCII or SPC trace file.

While in the File | Save Trace… dialog, simply check the Predict Header box in the frame Include with ASCII file.



Appendix C
Enhanced handling for SPC files

Four new File commands were added to enhance batch handling of saved SPC files.



1. **Interpolate SPC Files…**

   This utility function will re-interpolate any number of selected SPC files in a common directory. The SPC files will be re-interpolated to match the wavelength spread and step size of the *currently displayed graph*.

   When **Interpolate SPC Files…** is selected, the user is prompted to select the SPC files to re-interpolate. The chosen SPC files are permanently written with the new step size and wavelength spread.

2. **Average SPC Files…**

   This utility function creates a single SPC file that is the mathematical average of any number of SPC files in a common directory. *For this function to work correctly, the step size and wavelength spread must be identical for each of the selected SPC files.*

   When **Average SPC Files…** is selected, the user is prompted to select the SPC files to include in the average. Next, the user will be prompted to select a single destination SPC filename. If the file exists, the user will be warned before the file is overwritten.

3. **Save SPC Timestamp…**

   This utility command will extract the timestamp information from any number of SPC files and record the result in a selected tab delimited text file.

   When **Save SPC Timestamps…** is selected, the user will first choose a ___.txt filename to record the resulting table. A file dialog will then appear that allows the user to choose any number of SPC files from a common directory.

4. **Convert SPC files to ASCII…**

   This utility command will convert any number of binary SPC files selected from a common directory to ASCII text. The resulting ASCII files will be written to that same directory.

   When **Convert SPC Files to ASCII…** is selected, the user will be prompted to select the SPC files to convert. The function will then convert the files to ASCII.

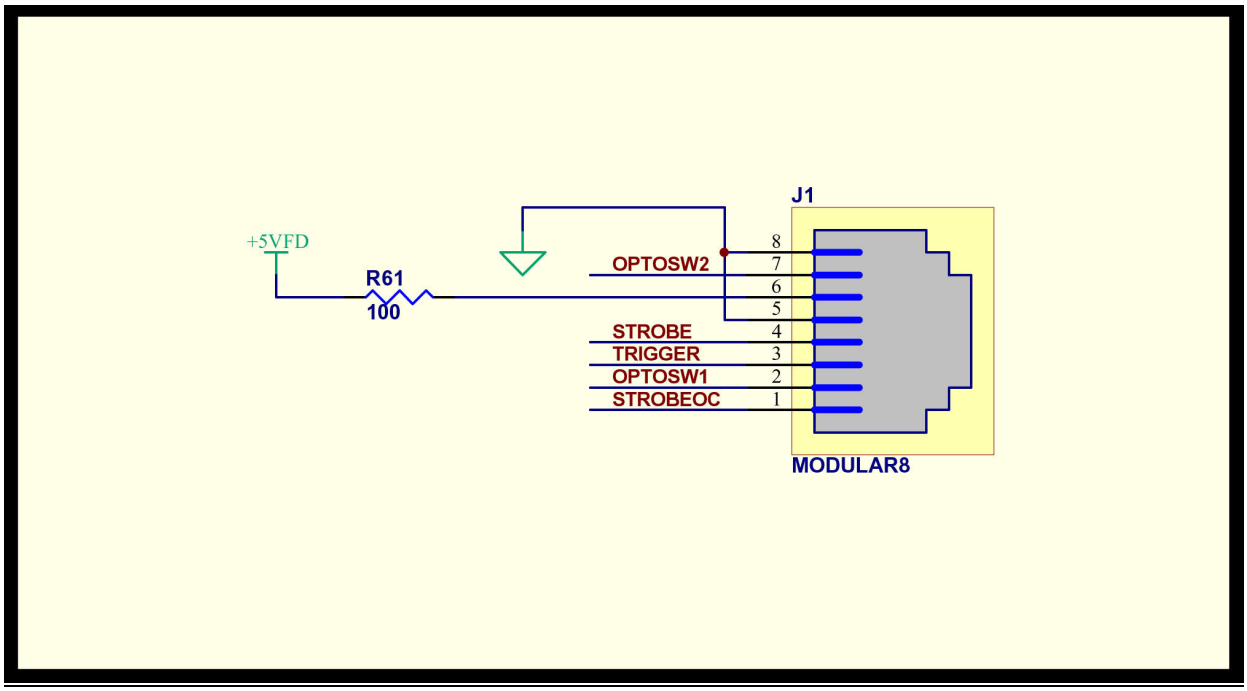
   The primary filenames will be retained, while the extension will change from ___.spc to ___.dat. Any header information that was saved in the SPC file will not be converted to the ASCII file. Also, if the ASCII filenames already exist, no warning will be issued before the files are overwritten.

A message box will indicate when the conversions are complete.

Appendix D
Pinout

1. Modular Electrical Connector Pinout

All spectrometers provide an I/O interface via an RJ45 connector. The user can connect to this interface by using a cable with a cable mount plug with the part number: AMP P/N 5-554739-3.



The following is a pinout description for this connector.

PIN	NAME	FUNCTION
1	STROBEOC	Output – Active during sampling, open collector output
2	OPTOSW1	Output – Engages / disengages a single fiber optic switch, 5V – 300mA Inductive load driver.

3	**TRIGGER**	**Input – Initiates a sample in manual mode, defines arrangement of sampled spectra in auto mode, +10V/-5V max. Input, +5V/0V nom.**
4	**STROBE**	**Output _ Active during sampling, TTL output.**
5	**GND**	**Ground – Return for all signals**
6	**PULL – UP**	**Power – 100 OHM resistor from internal +5V**
7	**OPTOSW2**	**Output – Engages / disengages a single fiber optic switch, 5V – 300 mA Inductive load driver (not available on CCD models)**
8	**GND**	**Ground – Return for all signals**

All Spectrometers can be fitted with a DB9 Electrical connector as shown below (order CDI TRIGGER CABLE). This utilizes a male DB9 connector and mates with an AMP P/N 747904-2 connector.

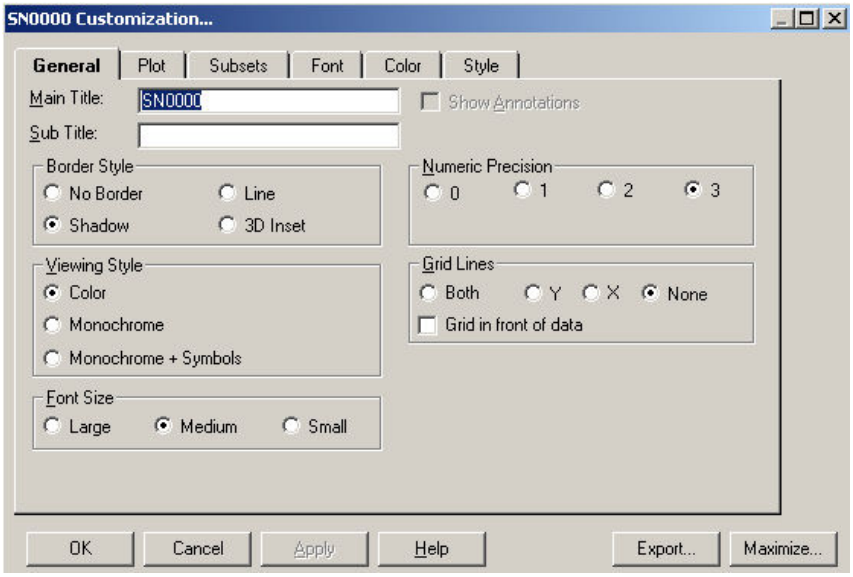
The following is a pin out description for this connector.

PIN	NAME	FUNCTION
1	**OPTOSW1**	**Output – Engages / disengages a single fiber optic switch, 5V – 300mA Inductive load driver. (NOTE: Tied to pin #2 on CCD adapters.)**
2	**PULL-UP**	**Power - 100 OHM resistor from internal +5V**
3	**GND**	**Ground – Return for all signals**
4	**GND**	**Ground – Return for all signals**
5	**OPTOSW2**	**Output – Engages / disengages a single fiber optic switch, 5V – 300mA Inductive load driver.(Not available on CCD models)**
6	**TRIGGER**	**Input- Initiates a sample in manual mode, defines arrangement of sampled spectra in auto mode, +10V/-5V max. input, +5V/0V nom.**
7	**STROBE**	**Output - Active during sampling, TTL output**

8	**STROBEOC**	**Output – Active during sampling, Open collector output**
9	**No Connection**	

Appendix E
Graph Appearance Customizations

Graph settings are customization options where many settings for the look and feel of the CDI Spec32 graph window can be changed. Examples of such settings are the font size, the background color, or turning grid lines on and off… See the Appendix for a detailed description of the options available.



To use this command, click on **Setup** on the menu bar, and select **Graph Settings.** A small windows dialog comes up. There are six tabs at the top of the window. The **General** tab is the default tab.

Note: Double clicking on the graph window will also have same effect as using the **Graph Settings** command.

1.1. General

1.1.1. Main Title and Sub Title

These two edit-boxes allow adding, editing, and deletion of main and sub titles. If no title is present, entering one will add one. If you remove all the characters from a title it will be deleted from the image.

1.1.2. Border Style

There are four radio buttons in this group, and only one can be selected at a time.

(a) No Border: No border will be drawn on the graph
(b) Shadow: A line will be drawn a round graph with drop shadow that will give the impression that graph is floating.
(c) Line: A line will be drawn around the graph.
(d) 3D Inset: A sunken border will be drawn around graph that gives a three dimensional look.

1.1.3. Viewing Style

The Graph Object supports three viewing styles.

- Color
- Monochrome
- Monochrome with Symbols

This customization allows you to quickly adjust the image to best suit printing on a monochrome printer. If fewer than four subsets are to be included in a graph, then the Monochrome setting will likely be the best choice. If four or more subsets are to be included in the graph, then Monochrome with Symbols will help distinguish the different subsets.

1.1.4. Font Size

The Graph Object supports three font sizes: Large, Medium, and Small. Depending on the size of the graph, the user can select the font size that is most readable. When printing the graph, a font size of Medium or Small is suggested.

There are occasions, (mainly when attempting to generate an image for a highly rectangular graph) the graph may automatically reduce the size of the font in order to produce a higher quality image.

1.1.5. Show Annotations

If the object contains annotations, this check box allows you to remove/add the annotations from the image.

1.1.6. Numeric Precision

When placing information into a table, or exporting Text/Data from the Export Dialog, the number of decimal positions can be between 0 to 7. Depending on the implementation, the maximum precision may vary.

1.1.7. Grid Lines

The Graph Object can contain vertical grid lines, horizontal grid lines, both vertical and horizontal grid lines, or no grid lines.

1.1.8. Grid in front of data

By checking this option, the graph's grid is placed in front of the data graphics. Otherwise, the data graphics are drawn on top of the graph's grid.

1.2. Plot

1.2.1. Plotting Method

The Graph Object has many possible plotting methods for the primary plotting style:

- Area
- Bar
- Line
- Point
- Points plus Best Fit Curve
- Points plus Best-Fit-Line
- Points plus Spline
- Spline

Depending on the implementation, some plotting methods may not be available. Also, many but not all of these plotting styles can be set for a secondary comparison plotting style.

If the graph has multiple y-axes, then you can control plotting and comparison plotting styles for each individual axis by selecting the axis in the axis-button group.

The Histogram plotting method displays a histogram of the data that is currently selected. The Histogram is most meaningful with larger data sets (at least 15 data points). If the Histogram is for only one subset, then bars represent the number of

occurrences. If the Histogram is for multiple subsets, then lines will represent the different frequency distributions.

1.2.2. 3D

This feature allows you to adjust 3D effects added to plotting methods. Possible values are:

None No 3D effect is added.

Shadows Draw shadows behind bars, points, and the area of an area graph.

3D Bars and area charts are drawn in a 3D fashion.

1.2.3. Mark Data Points

Checking this checkbox will cause little circular marks to be placed at data point locations.

1.3. Subsets

1.3.1. Subsets to Graph

This group allows you to view subset information is a variety of ways.

1. If nothing is selected in the listbox and Scrolling Subsets equals zero, then the object will display all subset information (14 subsets graph maximum, and no limit on the amount of subsets tabled.)
2. If there are selections in the listbox and Scrolling Subsets equals zero, then the object will display only those subsets selected.
3. If nothing is selected in the listbox and Scrolling Subsets is non-zero, then the object will scroll through subset information by the amount defined by Scrolling Subsets.
4. If there are selections in the listbox and Scrolling Subsets is non-zero, then the object will maintain those selected subsets as permanent subsets and revolve through the remaining subsets in increments of Scrolling Subsets.

The following table summarizes the Subsets to Graph variations.

Selected Subsets	Scrolling Subsets	Result

no	no	Display all subsets.
yes	no	Display only those selected subsets.
no	yes	Scroll through all subsets.
yes	yes	Permanent selected subsets & scroll through remaining subsets.

1.4. Fonts

The Scientific Graph Object only supports True Type fonts (because they are scalable). Your can select fonts for the following categories:

- Main Title
- Sub Title
- Labels, including the X axis, Y axis, X axis grid numbers or point labels, and Y axis grid numbers.
- Tabled Data Data labels included into the graph.

For the Main Title, Sub Title, and Labels, you can also select font attributes of Boldness, Italics, and Underline.

1.5. Colors

The Scientific Graph Object supports two sets of color parameters. A Monochrome color set and a Color color set. Depending on the Viewing Style, the Colors Dialog will customize the appropriate set.

To adjust the colors:

1. Select the desired object attribute in the Graph Attributes section. The corresponding color for that attribute will be highlighted in the color selection grid.

2. To change the color, either use the mouse to click an alternate color, or use the keyboard arrow keys to move to adjacent colors. As the highlighted color selection changes position, the sample image will be updated with the newly selected color.

3. Finally, Pressing the OK button will update the color parameters of the object.

1.5.1. Desk Background

This is the color that surrounds the bounding rectangle of the graph's grid.

1.5.2. Desk Foreground

This is the color that is used when placing text onto the Desk Background. This includes the main title, sub title, subset labels, grid numbers, and axis labels.

1.5.3. Shadow Color

The rectangle that make up the graph's grid is bounded at the bottom/right edges with shadows. To remove the shadows, choose the same color as the Desk Background.

1.5.4. Graph Background

This is the color used as the background color of the graph's grid.

1.5.5. Graph Foreground

This is the color used for the bounding rectangle of the grid, and the grid-lines.

1.6. Style

The Style tab allows the control of subset color, subset line style, and subset point style.

1. Select the desired subset in the Subsets list box. The corresponding color and possible line and point styles are then highlighted in their respective controls.

2. To change the color, either use the mouse to click an alternate color, or use the keyboard arrow keys to move to adjacent colors. Adjust the subset line and point styles as desired.

3. Finally, Pressing the OK button will update the object's image.

1.7. Customization Dialog Buttons

1.7.1. Customizations

All objects have their own individual customization dialogs. The customization dialogs allow you to adjust visual, and functional attributes of the object as well as gain access to the Export and Maximization dialogs.

Custom and Original Parameters

All objects store two sets of customization parameters. The first set is known as the Original set. The Original set is programmed into the control and you cannot adjust these parameters. The second set is called the Custom set. The Custom set can be adjusted through the customizations dialog. While the object has the input focus, PRESSING T will toggle between the Original and Custom parameter sets.

Showing the Customizations Dialog

DOUBLE-CLICKING the MOUSE over the object, or PRESSING SPACEBAR while the object has the input focus will show the customization dialog.

How to

When the customization dialog is shown, the parameters it shows reflect the current state of the object. By making adjustments to the customization dialog and then pressing the **OK** Button, the user updates the Custom set of parameters controlling the object. By pressing the Original Button the object will show the object with the Original set of parameters.

The **Apply** button is similar to the **OK** button but does not close the customization dialog.

The Color Tab and Font Tab allow adjustment of color and font attributes. To change colors or fonts, press the tab to show the dialog, make your adjustments and then press the **OK/Apply** Button to update the image.

Note, the customization dialog cannot be used to toggle between the Original and Custom set of parameters. This is because pressing the **OK Button creates a new Custom set of parameters. To toggle between Original and Custom sets of parameters, press the T key while the object has the input focus.

1.8. Exporting

All objects have the same exporting capabilities. Objects can export the following formats to the listed destinations.

FORMAT	DESTINATIONS
Metafile	Clipboard, File, and Printer.
Bitmap	Clipboard, and File.
OLE Object	Clipboard. (16 bit only)
Text / Data	Clipboard, and File.
JPEG	File.

How to

By Pressing 'X' when the object has the focus, or selecting the Export button from the Customizations Dialog.

1. Select the type of export desired.
2. Select the destination of the export.
3. If available, select the size of the image to export.
4. Press the Export/Print button.

1.8.1. File Destination

If information is to be exported to a file, then you must enter a target filename. Click the mouse over the **Browse** button to show the **File Save As Dialog**. Enter a filename and select **OK** to close the **File Save As dialog.**

1.8.2. Printer Destination

If you're exporting a metafile to the printer, pressing the **Print** button will show the **Print Dialog**. Use the Print Dialog to make changes to the selected printer, orientation, paper bin, and other printer options.

1.8.3. Exporting Text /Data

When exporting Text/Data, pressing the Export button launches the **Text/Data Export Dialog.**