



a subsidiary of EIC Laboratories, Inc.

**RS2000-3B
RAMAN SPECTROMETER**

USERS' MANUAL
(VERSION 2.1)

RS2000-3b-785
RS2000-3b-532
RS2000-3b-670

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I. System Overview

The RS2000 Raman spectrometer system is a fiber optic Raman spectrometer based on an echelle spectrograph. Because there are several variations of the system, it is important to understand the system configuration prior to use. The model number indicated on the identification label can be used to identify the system configuration.

Example: Model Number RS2000-AA-XXX

As shown above, the model number includes two variables: AA defines the laser class number (indicated by “1” or “3b” for a Class I or Class IIIb system), and XXX defines the excitation laser wavelength (either 532, 670, or 785 nm).

This manual describes the safety, operation, maintenance, and service procedures for the RS2000-1-XXX models. If your system identification label indicates otherwise, please consult InPhotonics for the appropriate manual.

A. RS2000 System Components

The RS2000 Raman spectrometer system consists of two separate units and requires a PC data station for data acquisition. The general layout is shown in Figure I.1.

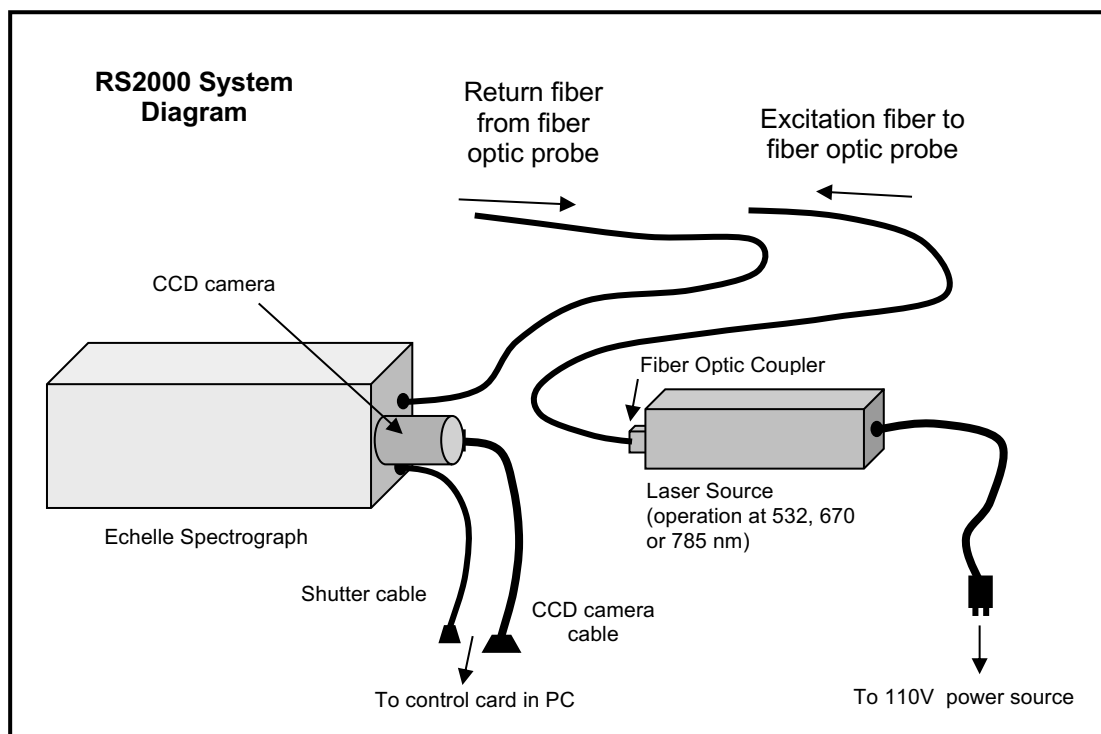


Figure I.1. Schematic diagram of RS2000-3b-XXX Raman spectrometer system components.

The laser source (operating at a single wavelength in cw mode) is connected to a 110V power source. At the laser head, a fiber optic coupler is attached. An excitation fiber optic cable from a fiber optic probe is connected to the laser source. The return fiber optic cable is connected to the echelle spectrograph. Inside, the spectrograph, the Raman scattered light is dispersed and imaged onto a CCD array inside the camera. The signal from the camera is transferred to the data card inside the PC data station (provided with the system or supplied by the user). Electrical power to drive both the CCD camera and the mechanical shutter in front of the camera are obtained directly from the PC via the data card provided with the camera.

Further information about each component is provided in section I.C.

B. Laser Safety

Note: The Model RS2000 Raman spectrometer system can be used with the following laser sources: 532 nm (up to 150 mW), 670 nm (up to 150 mW), 785 nm (up to 300 mW). Depending upon the system configuration (as described by the Model Number explained in Section I), the laser class is either Class I or Class IIIb. **VERIFY THE MODEL NUMBER INDICATED ON THE PRODUCT IDENTIFICATION LABEL TO ENSURE THAT THE PRODUCT FALLS INTO THE CLASS IIIb CATEGORY AS DESCRIBED IN THIS MANUAL.**

In some cases, the echelle spectrograph and fiber optic probe may be supplied for use with a customer-supplied laser system. In this case, the customer should verify the safety class of the laser source (as indicated by the warning logotype on the laser and described in the laser manufacturer's manual). Based on the laser source, the class of the spectrometer system should be determined and appropriate safety measures should be undertaken.

The Model **RS2000-3b-XXX** Raman spectrometer system can be used with the following laser sources: 532 nm (up to 150 mW), 670 nm (up to 150 mW), 785 nm (up to 300 mW). During normal operation and maintenance, the system is a CLASS IIIb product.

CAUTION

The use of controls and adjustments, or performance of procedures other than those specified herein may result in hazardous laser radiation exposure.

The RS2000-3b-XXX spectrometer systems are Class IIIb products. During normal operation, laser radiation is accessible from the end of the fiber optic coupler or any attached sampling probe. The output energy should be enclosed whenever possible (using the beam attenuator provided) to avoid unnecessary exposure. The laser source should also be turned off when the system is not in immediate use.

AVOID DIRECT EXPOSURE TO THE LASER BEAM

The laser sources supplied with the RS2000-3b can be connected to a remote interlock for an additional safety feature. A sampling device that incorporates a fiber optic probe can be constructed to be a Class I product with such an interlock. The door to the laboratory where the RS2000-3b is installed can also be connected to the remote interlock. Since the interlock connection is accessible directly from the laser system, consult the laser manufacturer's manual for connection instructions.

The RS2000-3b-XXX Raman spectrometer complies with "Performance Standards for Laser Products", United States Code of Federal Regulations, 21 CFR 1040.10 and 21CFR 1040.11.

The product falls into Class IIIb, and the appropriate warning labels are attached to the system (Figures 2 and 3). Prior to initial operation, annually, or whenever the product has been exposed to adverse conditions, the user should have a factory-trained service person verify the following to maintain compliance:

1. Verify the integrity of the fiber optic cable.
2. Inspect all protective housings for possible adverse wear.
3. Inspect the condition of all protective housing labels.
4. Verify the operation of all emission indicators.

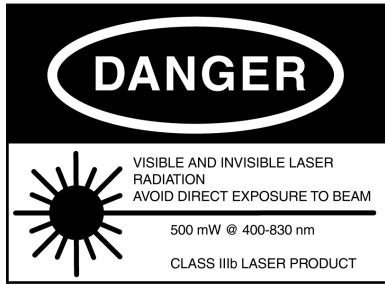
A source for additional information on laser safety is:

“American National Standard for Safe Use of Lasers” (Z136.1)
American National Standards Institute (ANSI)
11th West 42nd Street
New York, NY 10036

Precautions for Safe Operation of the Laser System:

- Do not, under any circumstances, remove the protective housing covers.
- Do not, under any circumstances, operate the system with the protective covers removed.

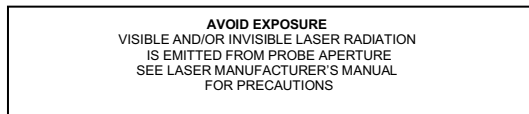
Figure 2: RS2000-3b-XXX Labels



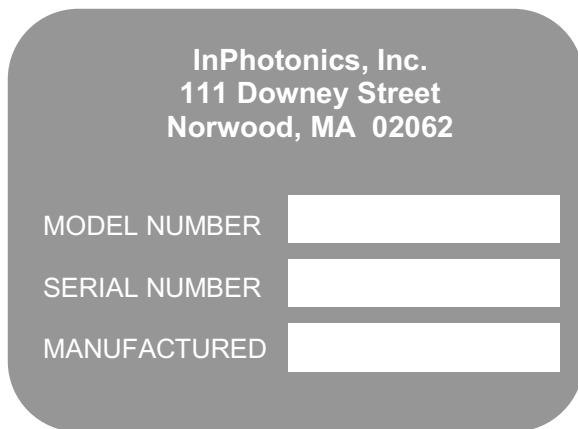
Class IIIb Warning Logotype



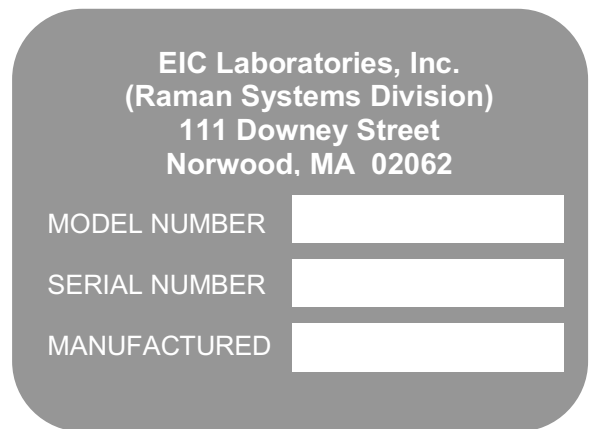
Protective Housing Label for non-interlocked protective housing



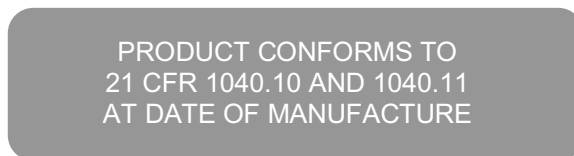
Aperture Label



Identification Label
(for products marketed by InPhotonics, Inc.)

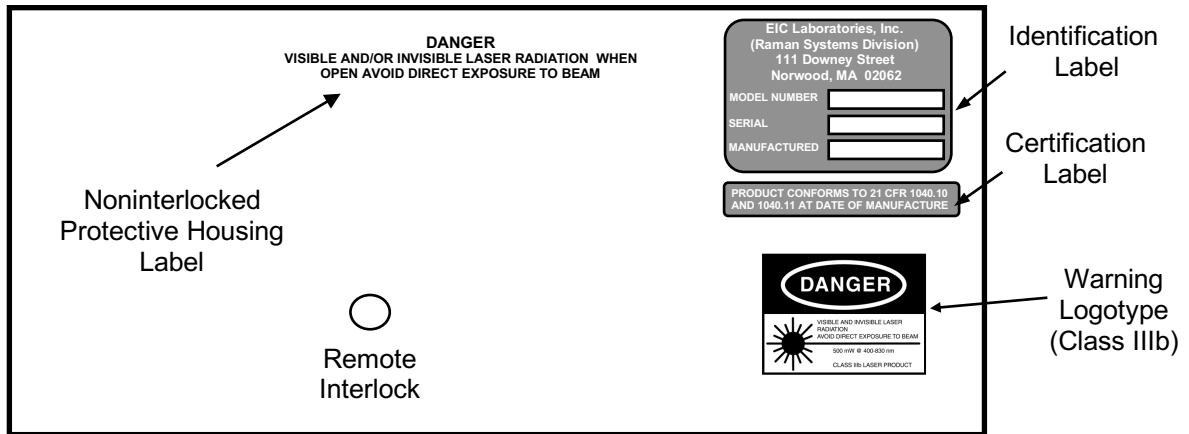


Identification Label
(for products marketed by EIC Laboratories, Inc.)

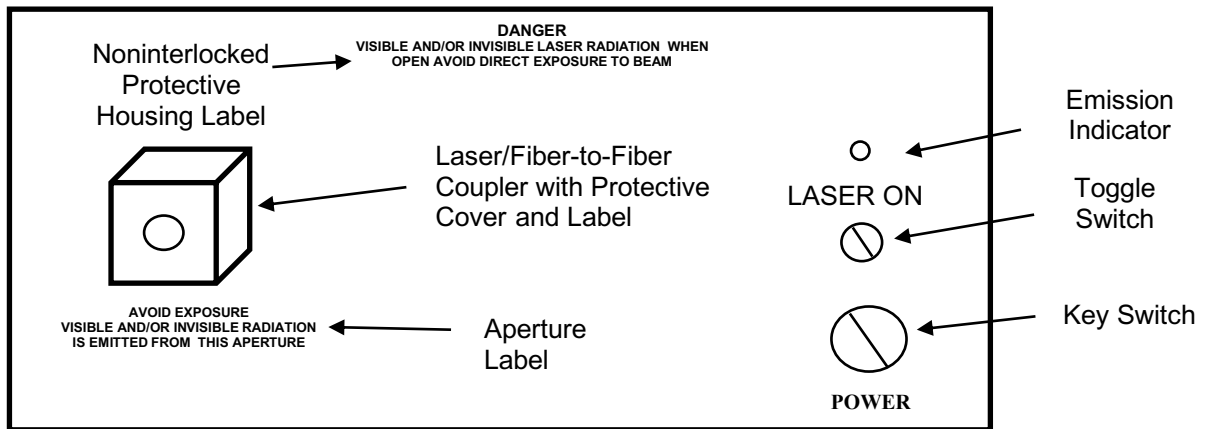


Certification Label

FIGURE 3: RS2000-3b-XXX
Location of Labels on Laser System



Rear Panel



Front Panel

C. Component Overview

1. Echelle Spectrograph

The InPhotonics echelle spectrograph is a specially designed unit that enables the end user to obtain the full Raman spectrum simultaneously while maintaining high resolution. Coupled to a fiber optic Raman probe, Raman spectra can be obtained rapidly by non-specialists through the use of a few simple computer keystrokes.

The echelle spectrograph is able to concentrate most of the available light into multiple coincident spectral orders with high dispersion. The multiple spatially overlapping orders are separated by a predispersion element and projected as stacked segments onto the focal plane. Utilization of a two dimensional charge coupled device (CCD) detector with the echelle theoretically allows the simultaneous acquisition of a complete ($0\text{-}4000\text{ cm}^{-1}$) Raman spectrum in a single measurement. The echelle spectrograph is designed to have minimal optical aberrations so that the resolution of the system is limited only by the entrance aperture and the CCD pixel element density. For the current application where the sample is remote from the Raman system, the optical fiber core serves as the limiting aperture.

A schematic of an NIR echelle unit is shown in Figure I.4 for the near-IR and visible echelles, respectively. A 50 to 200 μm core fiber optic from the Raman probe with FC connectors is coupled to the fiber optic entrance port of the echelle. The light entering the spectrograph from the optical fiber is collected and collimated by a $f/2.0$ lens for the near-IR echelle and a $f/2.8$ lens for the visible echelle.

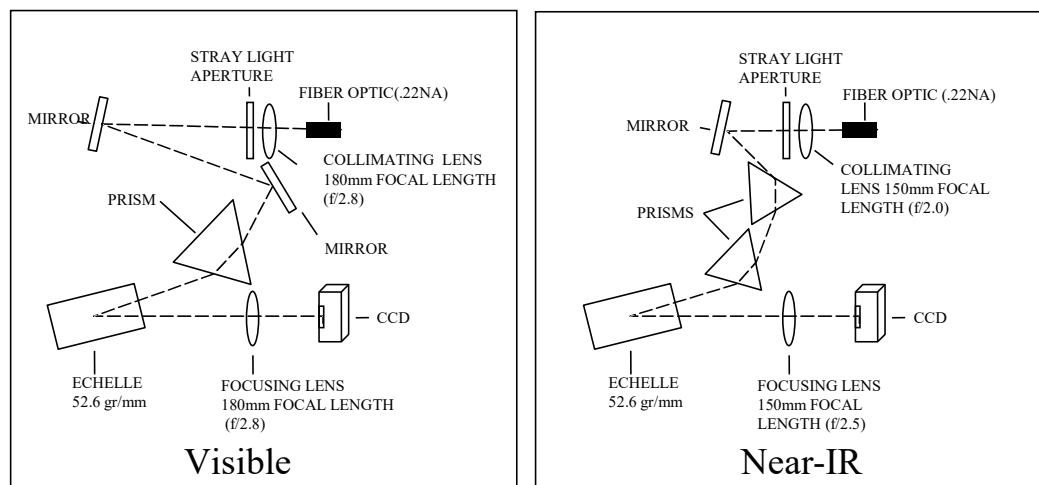


Figure I.4. Schematic diagram of a visible and NIR Raman echelle spectrograph.

Between the fiber optic and the lens is an electronic shutter that allows Raman signals to enter into the echelle when desired. The collimated light passes through a mask (stray light aperture) to remove unwanted background scattered light. The collimated light is then

reflected off a pair of turning mirrors into the prism before being dispersed into different orders by the echelle grating. In the near-IR echelle, the two dimensional array of collimated light is focused by a f/2.5 lens onto the CCD chip. With the visible echelle, the focusing lens is a f/2.8 lens.

The tilt of the echelle grating and the echelle spectral order range are determined by the wavelength of the light employed for the Raman scattering measurement. For excitation wavelength range of 750 to 785 nm, the echelle orders collected are 45 through 33 (742 to 1027 nm). On the other hand, for a green excitation (514-532 nm), the echelle orders collected are 66 through 52 (510 to 650 nm). The lower number echelle orders have the largest Raman shift from the excitation frequency. The InPhotonics echelle spectrograph can theoretically collect from 0-3500 cm^{-1} in a single scan. In practice, filtering of the excitation line limits the collection range to 225-3500 cm^{-1} .

a) System Alignment

The InPhotonics echelle spectrograph was aligned, calibrated, and tested prior to shipping. The mounts in the echelle system are designed to withstand vibration and should not change alignment during shipping. The echelle system is calibrated using emission lines from mercury, neon, argon, krypton, and xenon lamp sources.

b) Hardware Installation

The InPhotonics echelle uses a CCD detection system with a separate data acquisition/controller card. Proper operation of the detector and software requires a 486DX PC with at least 16MB Ram, a Bus Based Video Card and one PCI expansion slot. The expansion slot is used for the controller board for the CCD camera. The board is normally supplied preinstalled in the PC data station at the factory. If this is not the case, this board and the associated cables should be installed according to procedures described in manual provided by the CCD camera manufacturer. The operational temperature of the CCD camera is factory set for optimum performance near -50.0°C. **Please note that the cooling fan power supply must be on when operating the CCD. Operation of the CCD camera without the fan on can result in damage to the detector head.**

2. Laser System

The RS2000 systems are supplied with a Class IIIb laser system. The laser system is supplied with a fiber optic coupler (FC type) for the attachment of a fiber optic probe. Consult the laser manufacturer's manual for information on operation of the laser system.

3. Fiber Optic Sampling Probe

Models RS2000-3b-XXX are supplied with fiber optic couplers on the laser system and the echelle spectrograph for the attachment of a fiber optic sampling probe. The excitation cable

is connected to the laser system, and the collection cable is connected to the fiber optic input on the echelle spectrograph.

A fiber optic sampling probe enables the laser light to impinge on the sample of interest and transfer the Raman scattered radiation to the spectrograph for subsequent dispersion and detection.

4. PC Data Station

The RS2000 spectrometers require a PC data station for camera control and data acquisition. Consult the CCD camera manufacturer's manual for data station requirements.

II. RS2000 Instructions (Class IIIb Models)

CAUTION

The use of controls and adjustments, or performance of procedures other than those specified herein may result in hazardous laser radiation exposure.

Laser powers up to 500 mW at 785 nm, 300 mW at 670 nm, and 150 mW at 532 nm are be accessible from the fiber optic coupler.

AVOID DIRECT EXPOSURE TO THE BEAM.

A. Initial Setup and Installation

The Model RS2000-3b-XXX Raman spectrometer systems are designed to be installed only by InPhotonics certified technicians. Installation by anyone other than InPhotonics certified technicians may result in hazardous radiation exposure. Please contact InPhotonics to install your RS2000-3b-XXX system.

B. Basic Operation Procedures

(Please refer to the instructions supplied with the fiber optic sampling probe, if any, for operating procedures of the specific sampling accessory.)

1. Startup and Sample Measurement

1. Plug power cord of the laser system into a properly rated 110V outlet. The keyswitch should be in the “OFF” position.
2. Verify that a beam attenuator is installed on the fiber optic probe, or have the probe rigidly mounted (e.g. with a clamp) such that the laser radiation is pointed only on the sample of interest.
3. Turn the laser system keyswitch to the “ON” position. The emission indicator on the laser system will start after a short delay to indicate that the laser is emitting radiation.
4. Remove the beam attenuator on the fiber optic probe (if necessary) and adjust the position such that the laser beam is focused onto the sample of interest according to the manufacturer’s instructions. **Avoid direct exposure to the beam.**
5. Acquire the spectrum (see software section)

6. Repeat step 4 for remaining samples.

2. Shutdown Procedure

1. Turn the laser system keyswitch to the “OFF” position.
2. Replace the beam attenuator on the fiber optic probe.

C. Maintenance Procedures

WARNING

The laser portions of the RS2000 systems are designed to be maintenance free and should not be opened or adjusted by anyone other than InPhotonics certified technicians.

CAUTION

Opening of laser protective housings may result in exposure to hazardous laser radiation (up to 500 mW) and/or dangerous voltages. Please contact an InPhotonics representative for any maintenance or service of the laser systems.

Annually, it is recommended that a factory-trained service person verify the following to maintain compliance with “Performance Standards for Laser Products”, United States Code of Federal Regulations, 21 CFR 1040.10 and 21CFR 1040.11:

1. Verify the integrity of the fiber optic cable.
2. Inspect all protective housings for possible adverse wear.
3. Inspect the condition of all protective housing labels.
4. Verify the operation of all emission indicators.

D. Troubleshooting

If the laser fails to turn on after following the start-up procedures, turn the keyswitch to the “OFF” position, then:

1. Check that the power cables and/or circuit breakers are operational.
2. Check the line voltage fuse.

If, after checking steps 1 and 2, the laser emission indicators do not illuminate, contact the laser manufacturer or InPhotonics for service assistance.

E. Service Procedures

CAUTION

All service is to be conducted by factory trained personnel wearing eyewear appropriate for the laser system wavelength.

Laser powers up to 0.5W at 785 nm, 0.3 W at 670 nm, and up to 150 mW at 532 nm are accessible from the fiber coupler, and could also be accessible if the protective housings are removed and the laser systems are operational. The latter conditions should exist only during service by factory trained technicians and are outlined as follows:

1. Focused green (532 nm) is present in the fiber interface. It could be accessible during service if the beam cap was unscrewed from the coupler during the installation of a fiber optic probe.
2. Focused red (785 or 670 nm) is present in the fiber interface housing. It could be accessible during service if the beam cap was unscrewed from the coupler during the installation of a fiber optic probe.

III. Molecue Software Instructions

A. Software Installation

The RS2000 Raman spectrometer uses the following software systems that need to be installed on a x86 family PC with 16MB Ram, and One Expansion Slot:

GRAMS/386™ or GRAMS/32™ - Galactic Industries, Inc.
Molecue – InPhotonics, Inc.

The Molecue software controls the Andor CCD camera, and also calibrates, splices, and convert the echelle spectrum into a GRAMS/386™ or GRAMS/32™ file format. Proper operation of this software requires an Andor camera controller board to be installed in the system computer.

If the software has not been preinstalled, then perform the following installation procedures:

3. Install the GRAMS™ software first as described in the installation procedure in the GRAMS™ Manuals.
4. Once GRAMS™ is installed make sure that the Auto DDE Server mode is on under the Parameter.
5. Next, install the Molecue software using the specifically marked Molecue software diskettes.
6. Install the Molecue software, following the procedure in the following section.

1. Installation Procedure for the Molecue Program

The host computer should be a 486 or better IBM-compatible with at least 16 megabytes of RAM. Load a display driver (for your particular graphics card) capable of 256 colors at a resolution of 800 x 600. The indicated directory creation and file copying operations can be accomplished from Windows Explorer.

Load the main program & support files

1. Create the directory c:\InPhotonics
2. Load the following files into c:\InPhotonics:

| | | | |
|--------------|--------------|--------------|-------------|
| Molecue.exe | InPhotc2.bmp | inphoton.ips | rd*****.ipc |
| Detector.ini | Wct32fr3.dll | Atmcd32d.dll | Pci_29k.cof |
| Pci_fpga.rbf | Molecue.hlp | Molecue.cnt | white.spc |

*.ipc (calibration file name)

Create the Molecue.exe Shortcut on the desktop

1. From the File menu in Program Manager, choose Start, then Programs, and finally Windows Explorer.
2. Select the Program Molecue.exe and drag it onto the desktop then OK.

Run Molecue Program

1. Double-click the Molecue icon on the desktop.
2. Molecue should start (perhaps taking several seconds to load and set up).

Changing the Calibration File and Startup Parameters for the Molecue Program

To change the ***calibration file, laser wavelength, camera ID or the initial plot limits*** on startup, you must run the InPhoHdr.exe program. The InPhoHdr program makes changes to a file named inphoton.ips. Any changes made to the parameters must be stored under the file name inphoton.ips to take effect. See later section for more details about InPhoHdr.exe.

B. Software Features

In the Molecue software, spectra can be acquired, viewed, and stored in a compact format. Key molecue software features utilized with the InPhotonics echelle will be discussed here.

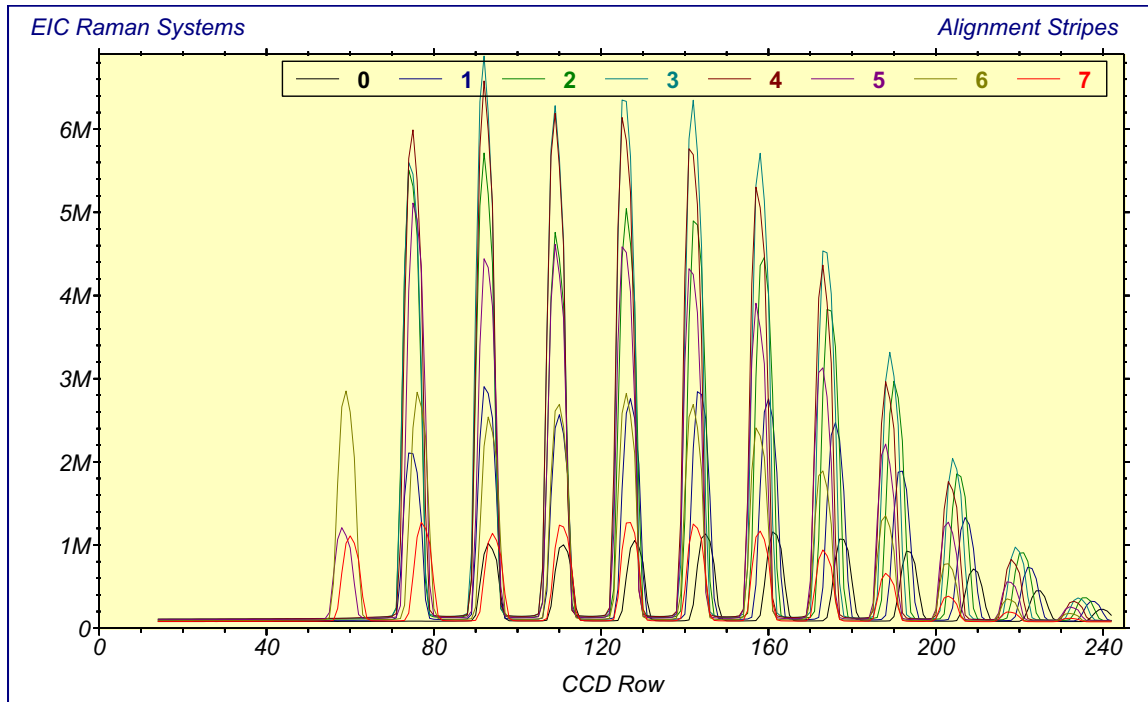
1. Molecue Graph Types

Molecue can display six distinct graphs. The purpose of each should be understood by the user. The six supported graph types are:

Alignment: The Alignment graph is provided as a check on the alignment of the track/camera/spectrograph combination. Eight (8) plots are displayed on the Alignment graph. Each plot represents the intensity of a vertical stripe as a function of row number. The Alignment graph is used only for initial setup or service and is not used during normal operation.

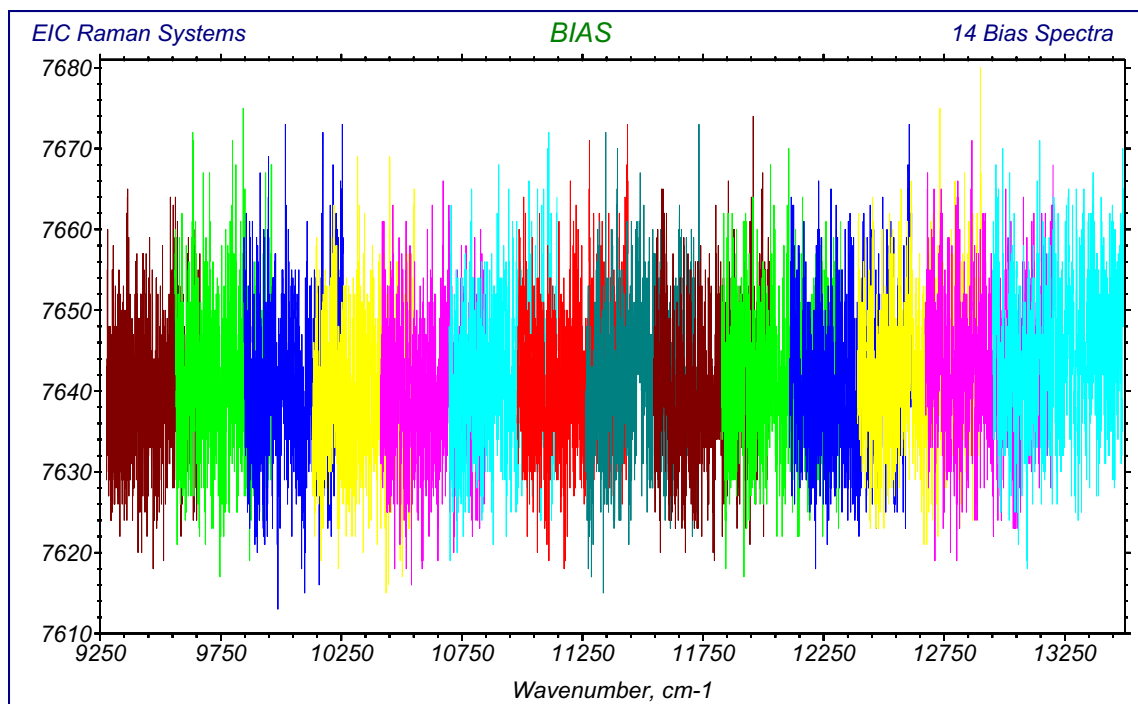
Alignment

(Used only for initial setup or service.)



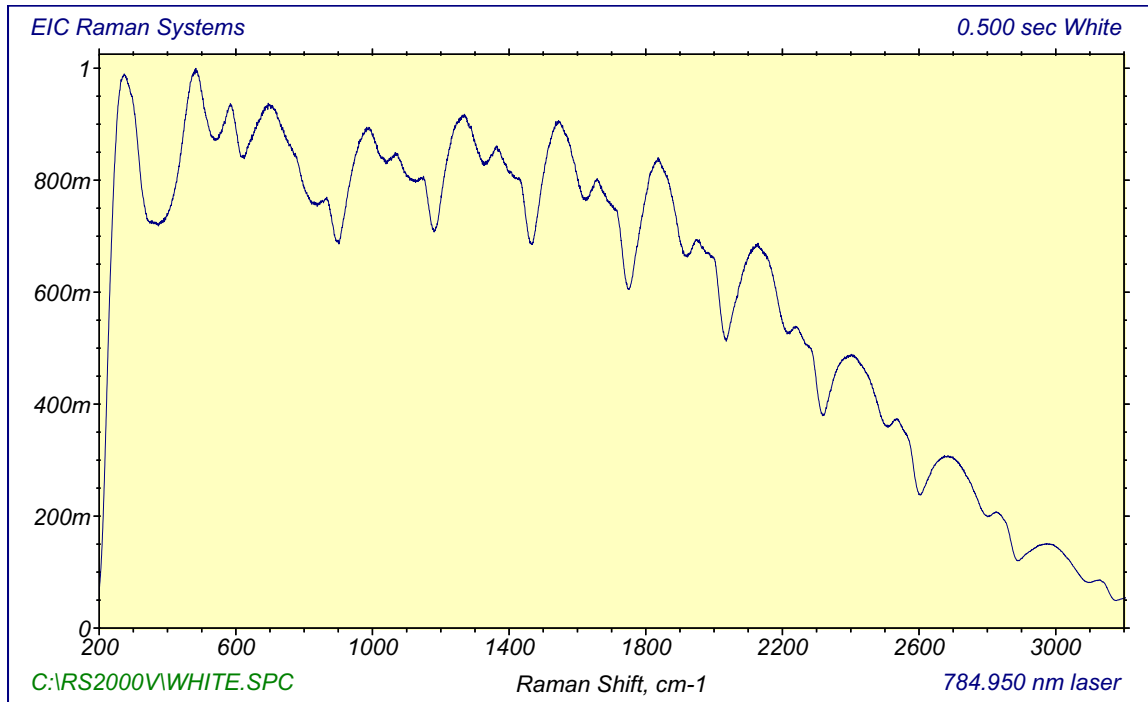
Bias: The Bias graph appears whenever a bias spectrum is acquired. A bias spectral acquisition is performed using a zero-second exposure time for the CCD camera without opening the shutter. The Bias graph displays the intensity of each track as a function of absolute wavenumber. There are as many plots (distinguished by color) on the Bias graph as there are tracks defined for the system camera. The bias serves as an indicator of camera performance. The bias data is saved within the running Molecue program. There is no provision for saving or recalling bias data. However, The Bias plot can be saved in a Windows metafile if desired. The bias will change whenever the temperature of the camera changes significantly. A bias acquisition is performed automatically upon Molecue startup. **Note that the bias changes significantly with camera temperature. For this reason, a new Bias should be acquired when the camera reaches its equilibrium operating temperature.**

Bias
(Closed shutter, zero-time, track-by-track CCD readout.)



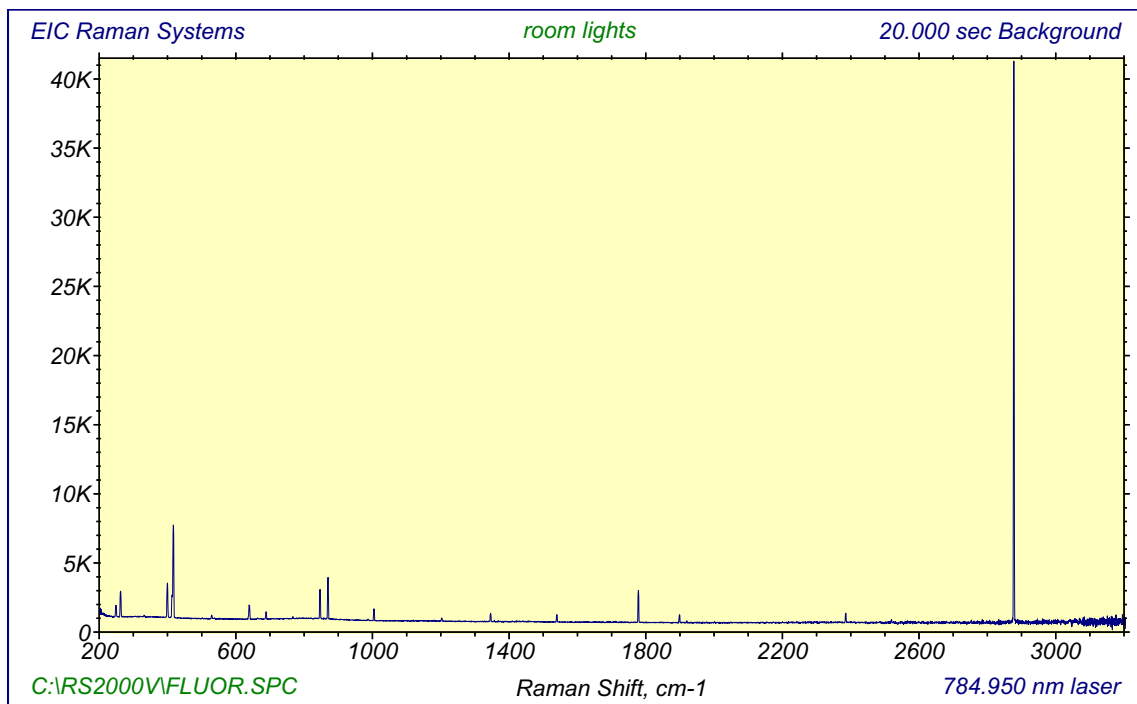
White: The White graph displays the White spectral intensity as a function of Raman-shifted wavenumber. The White spectral data is essential to the acquisition of meaningful Raman spectra. It is used as a means for correcting for the response characteristics of the probe, the spectrograph, and the CCD camera. The White spectrum is displayed in normalized form with a range of zero to unity. A White spectrum should be acquired from a white light source through the probe with a short exposure time. It is essential that cosmic occurrences or saturation of the CCD not be in the White spectrum. Normally, a White spectrum is acquired once, stored to a file (with filename **WHITE.SPC**), and recalled automatically upon system startup.

White
(White light spectrum to define system response function.)



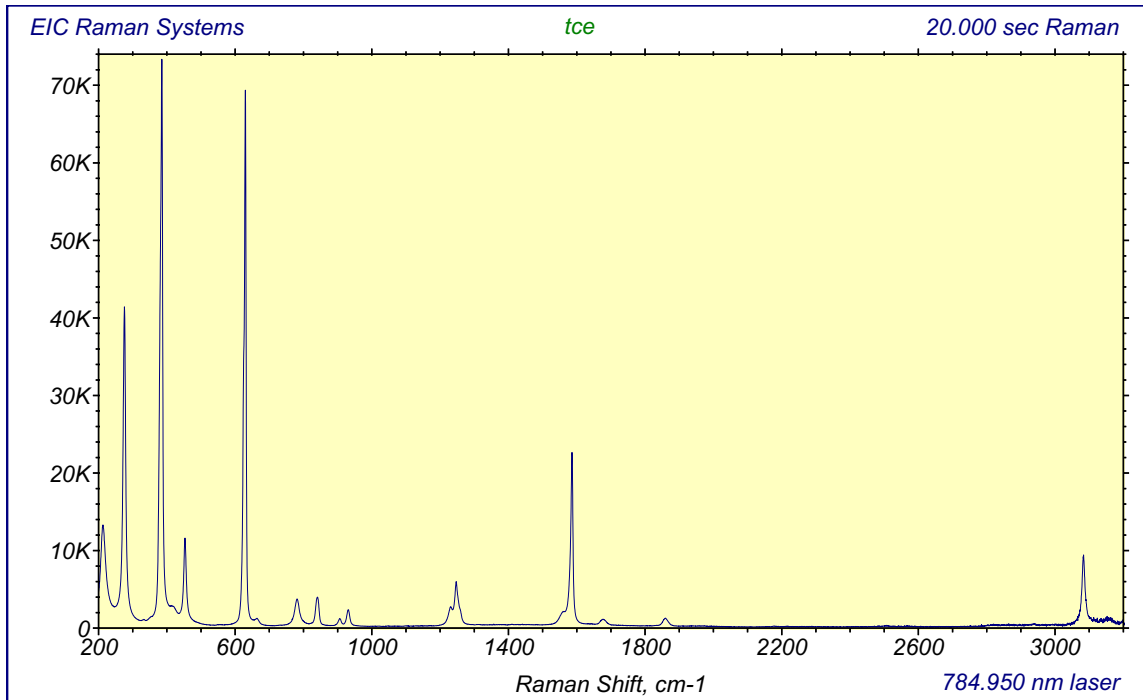
Background: The Background graph displays the Background spectral intensity as a function of Raman-shifted wavenumber. If Background Removal is toggled OFF, the Background spectrum has no effect on the Raman spectrum. If Background Removal is toggled ON, the Background spectrum is subtracted from the Raman spectrum before the Raman spectrum is displayed. Background use is optional.

Background
(Spectrum for Background removal.)



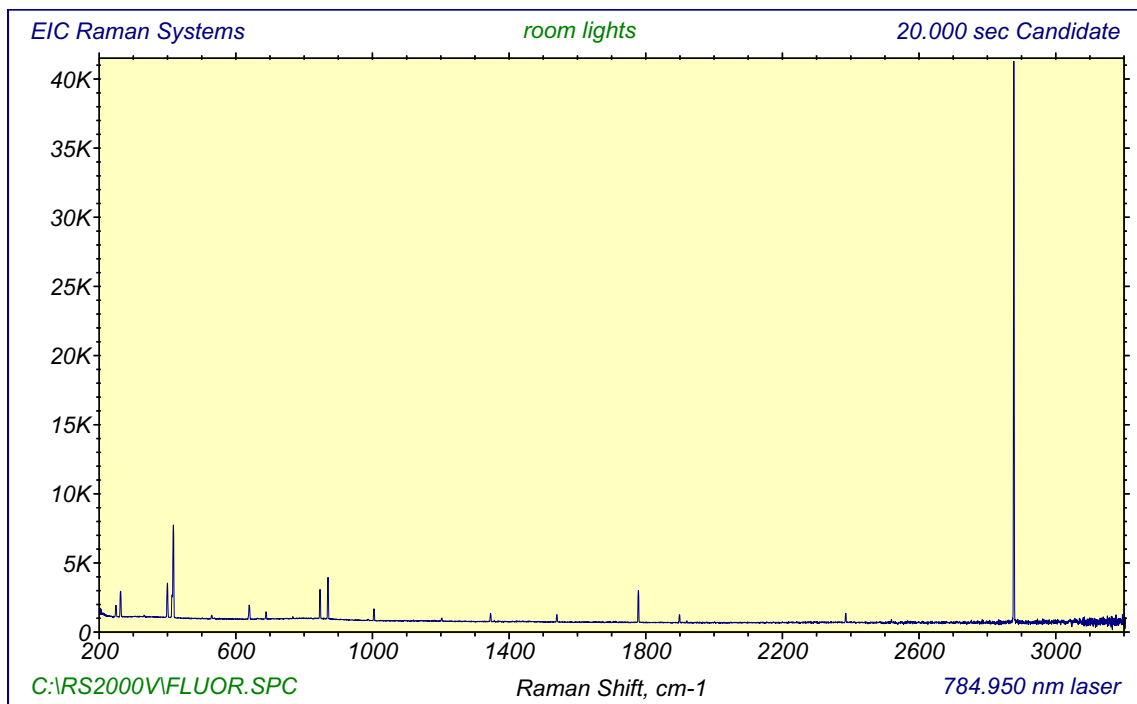
Raman: The Raman graph displays the Raman spectral intensity as a function of Raman-shifted wavenumber. If Background Removal is toggled ON, the Background spectrum is subtracted from the Raman spectrum before the Raman spectrum is displayed. NOTE: Once the Background spectrum has been subtracted from the acquired spectrum and displayed as a Raman spectrum, the removed spectral information cannot be restored within Molecule.

Raman
(Sample spectrum (w/ or w/o Background removal.)



Candidate: The Candidate graph is provided as a utility for spectral acquisition and recall. Candidate data is valid only when the Candidate graph is displayed. For this reason, there is no provision for returning to the Candidate graph without overwriting its data. The Candidate appears under three circumstances. Whenever spectral data is recalled from a file, the corresponding spectrum is temporarily displayed as a Candidate graph. Upon switching to White (or Background), you will be prompted for the choice of overwriting the currently stored White (or Background) spectrum. Whenever a White or Background spectrum is acquired, the spectral data is initially stored in the Candidate. Molecue will then prompt you to overwrite the previous (White or Background) spectrum.

Candidate
(Temporary (acquisition or file recall) spectrum.)



2. Summary of Controls

Main Menu (“InPhotonics-Molecue” Window)

| MENU ENTRY | <i>RESULTING ACTION</i> |
|------------------------------|--|
| File | |
| <u>O</u> pen | Recall a spectrum from an spc file |
| <u>S</u> ave | Save a spectrum to an spc file.(GRAMS 386 format) |
| <u>P</u> rint | Print the current Molecue graph. |
| Print <u>P</u> review | Screen preview of graphics output. |
| Print <u>S</u> etup | Configure the active Windows hardcopy device. |
| Save as <u>M</u> etafile | Save the current Molecue graph to a Windows metafile. |
| Background <u>R</u> emoval | Toggle removal of Background from Raman on/off. |
| <u>D</u> ark Removal | Toggle removal of Dark from Raman on/off. |
| <u>C</u> osmic Filter | Toggle application of Cosmic Filter on/off. |
| <u>A</u> lignment | Acquire an image and display an Alignment graph. |
| <u>R</u> ecalibrate vs. Lamp | Recalibrate the spectrograph (single track systems only) |
| <u>A</u> utodetect Camera | Detects camera ID address (installation/service only) |
| <u>E</u> xit | Close the Molecue program. |
| | |
| <u>E</u>xposure | Invoke the exposure time dialog box. |
| | |
| <u>S</u>pectra | |
| <u>B</u> ias | Acquire or access Bias spectrum. |
| <u>W</u> hite | Acquire or access White spectrum. |
| Background | Acquire or access Background spectrum. |
| <u>R</u> aman | Acquire or access Raman spectrum. |
| <u>D</u> ark | Acquire or access Dark spectrum. |
| | |
| <u>C</u>omment | Invoke the comment dialog box. |
| | |
| <u>H</u>alt | Terminate current spectral acquisition. |
| | |
| <u>G</u>rams/386 | Send current spectrum to GRAMS/386. DDE serve in GRAMS must be toggled on. |
| | |
| <u>L</u>imits | Set user-defined plot abscissa limits. |
| | |
| <u>V</u>iew | |
| Toolbar | Toggle the toolbar on/off. |
| Status Bar | Toggle the status bar on/off. |
| | |
| <u>H</u>elp | |
| About Molecue | Invoke the About Molecue dialog box. |

Toolbar

The Toolbar is a convenient means of accessing Molecue control operations. It is only a convenience. All Toolbar operations can be accessed through Main Menu entries or pulldown menus. The Toolbar buttons displayed are:



Open (same as File/Open) Recall a spectrum from an spc file.



Save (same as File/Save)
Save a spectrum to an spc file.



Exposure (same as File/Exposure) Invoke the exposure time dialog box.



Bias (same as Spectrum/Bias)
Acquire or access Bias spectrum.



White (same as Spectrum/White) Acquire or access White spectrum.



Background (same as Spectrum/Background) Acquire or access
Background spectrum.



Raman (same as Spectrum/Raman) Acquire or access Raman spectrum.



Halt Acquisition
Terminate current spectral acquisition.



Background Remove (same as File/Background Remove) Toggle removal
of Background from Raman on/off.



Filter (same as File/Cosmic Filter) Toggle application of Cosmic Filter
on/off.



Print (same as File/Print)
Print the current Molecue graph.



Metafile (same as File/Save Metafile) Save the current Molecue graph to a
Windows metafile.



Grams (same as File/Grams)
Send current spectrum to Grams/32



About (same as Help/About Molecue) Invoke the About Molecue dialog box.

NOTE: Molecue Controls are CONTEXT-SENSITIVE.

The same control action may produce different results if initiated under different circumstances. For example, if either File/Bias or the Bias Toolbar button control is selected, any of three actions may occur:

1. If there is not yet a bias spectrum in memory, a new Bias spectrum will be acquired and displayed.
2. If there is a Bias spectrum in memory AND the (preexisting) Bias spectrum is currently displayed, a new Bias spectrum will be acquired and displayed.
3. If there is a Bias spectrum in memory AND the (preexisting) Bias spectrum is NOT currently displayed, the preexisting Bias spectrum will be displayed.

At first, such context-sensitive controls may seem unnatural. However, the underlying logic is intended to permit examination of current Bias, White, Background, and Raman spectra while allowing spectral acquisition with a minimum number of keystrokes.

Special protection is afforded to preexisting White and Background data. Both White and Background acquire into the Candidate spectrum. An explicit operator decision is required to overwrite the Candidate or Background data.

Data is stored and recalled using the **Files** menu. The stored data in Molecue is in a standard SPC format (GRAMS/32™ software from Galactic Industries). Spectral manipulation is accomplished using GRAMS/32™ software from Galactic Industries. GRAMS/32™ is a sophisticated software routine that allows the end user to perform spectral subtraction, baseline correction, smoothing, spectral comparisons, spectral storage in a variety of user friendly formats, annotation of spectral data, and plotting of the spectral data. A more thorough discussion of the capabilities of GRAMS/32™ is done in the Galactic Industries manual.

C. Acquiring Spectra

Run the Molecue Program

1. Double-click the Molecue icon.
2. Molecue should start (perhaps taking several seconds to load and set up).

Acquiring BIAS Spectrum

Once the CCD has cooled to its operating temperature, Raman spectra may be collected with the RS2000 program. It is recommended that, prior to collection of Raman spectra, a Bias be collected and stored. The bias command is a record of the signal detected at the face of the camera when no light is present. In effect, it is a measure of the electronic noise of the camera. On the computer screen, the collected bias spectrum will appear as a noisy line in each echelle order. The bias is stored as a reference spectrum which allows for the subtraction of the electronic noise of the camera from the Raman spectrum. Collection and storage of the bias as the reference file is accomplished by clicking the mouse on the following toolbar icon:



Bias (same as Spectrum/Bias) Acquire or access
Bias spectrum.

Acquiring White Light Spectrum

During the collection of Raman signals a combination of several instrumental factors, including each echelle order efficiency, the efficiency of the edge filters as a function of wavelength, and the efficiency of the CCD detector as a function of wavelength may be observed. This "instrument factor" can be removed by normalizing the data against a white light efficiency spectrum. Thus, before acquiring Raman spectra with a new probe, a white light spectrum of the probe should be acquired and saved as **WHITE.SPC**. Normally, this is only done once for each probe. The white light spectrum corrects for instrument response function and probe function which are present in every Raman spectra acquired with the echelle system. A bias reference spectrum must be obtained first and automatically subtracted from the white light spectrum. Follow the procedure described above to obtain the bias spectrum.

A white light spectrum is obtained by shining a diffuse white light into the face of the Raman probe (note the excitation source should be **OFF**). A white light spectrum is accomplished by clicking the mouse on the following toolbar icon first to set the exposure time.



Exposure (same as File/Exposure) Invoke the exposure time dialog box.

Select an exposure time that will give a smooth spectrum *without* saturation occurring. The program will query you if saturation occurs. Then click the mouse on the following toolbar icon to acquire the white light.



White (same as Spectrum/White) Acquire or access White spectrum.

The program will query you as to whether to overwrite the existing white light spectrum or if saturation has occurred. **When an acceptable spectrum is obtained, it should be saved as WHITE.SPC.** Save the spectrum by clicking the mouse on the following toolbar icon.



Save (same as File/Save)
Save a spectrum to an spc file.

It should be noted that every time a new probe is connected to the echelle spectrograph, a white light spectrum must be obtained for the new probe and saved.

Acquiring Raman Spectra

Raman spectra are collected by utilizing the **Raman** option in the **Spectra** menu or by clicking the mouse on the toolbar icon. The exposure time should be set prior to clicking the Raman icon.



Raman (same as Spectrum/Raman) Acquire or access Raman spectrum (RED).

D. InPhoHdr Program for Echelle-based Raman Spectroscopy

InPhoHdr was developed to provide users access to system data for InPhotonics' spectral acquisition programs, specifically Molecue. The system file is named Inphoton.ips. Only this name will be detected by the Molecue spectral acquisition program. Inphoton.ips contains the IPS data structure in binary format. Any attempt to alter its data by programs other than InPhoHdr may result in data corruption that could render your spectral acquisition system inoperable until restored.

Run InPhoHdr Program

1. Open the InPhotonics folder
2. Double-click the InPhoHdr.exe icon
3. InPhoHdr.exe should start

To make any changes to the file

7. Click with the mouse IPS
8. Click Open
9. Double click Inphoton.ips
10. Edit the various parameters

To save any changes to the file

1. Click with the mouse IPS
2. Click Save
3. Double click Inphoton.ips

The editable data fields of the IPS data structure are:

Camera ID: The Camera ID is an integer flag for the address of the data acquisition card inside your computer. If this address is incorrect, the Molecue data acquisition program will be unable to access the CCD camera.

Laser Wavelength: The vibrational data comprising a Raman spectrum are displayed in terms of a wavenumber offset from the excitation laser. As such, any error in the wavelength of the excitation laser will cause an erroneous shift in the spectrum abscissa. The floating point laser wavelength is given in nanometers.

Lower Plot Limit: An Echelle spectrograph acquires data over a wide wavenumber range. You may prefer to limit the screen display of data to a narrower region. The lower plot limit is a user-defined value for the left side of the plotting abscissa. The floating point lower plot limit is given in wavenumber shift.

Upper Plot Limit: An Echelle spectrograph acquires data over a wide wavenumber range. You may prefer to limit the screen display of data to a narrower region. The upper plot limit is a user-defined value for the right side of the plotting abscissa. The floating point upper plot limit is given in wavenumber shift.

Banner: The banner appears in the Molecule plots. Altering this text string will change the banner displayed in the plots.

IPC Filename: The calibration data for your spectrograph is contained in a binary calibration file (*.ipc). This text string must contain the full path to the *.ipc calibration file. An example is "c:\InPhotonics\yourcal.ipc".

of Gratings: This integer value has no significance to your system.

Startup Grating: This integer value has no significance to your system.

1. InPhoHdr Summary of Controls

Main Menu (“InPhotonics-InPhoHdr” Window)

| <u>MENU ENTRY</u> | <u>RESULTING ACTION</u> |
|---------------------------|--|
| <u>F</u>ile | |
| <u>P</u> rint | Print the current InPhoHdr data. |
| Print <u>P</u> review | Screen preview of InPhoHdr data output. |
| <u>P</u> rint Setup | Configure the active Windows hardcopy device. |
| <u>E</u> xit | Close the InPhoHdr program. |
| <u>S</u>ystem | |
| <u>R</u> eset | Set IPS data to default values. |
| <u>E</u> dit | Edit IPS system data. |
| <u>O</u> pen | Open Inphoton.ips system file. |
| <u>S</u> ave | Save IPS data to inphoton.ips system file. |
| <u>C</u>alibration | |
| <u>R</u> eset | Set IPC data to default values. |
| <u>E</u> dit | Edit IPC system data. |
| <u>O</u> pen | Open IPC system file. |
| <u>S</u> ave | Save IPC data to IPC system file. |
| <u>S</u> hift | Shift the all tracks up (-) or down(+) by this number. |
| IPS to <u>E</u> IC | Convert from IPS (echelle) to EIC (InPhotote) format. |
| <u>V</u>iew | |
| <u>T</u> oolbar | Toggle the toolbar on/off. |
| <u>S</u> tatus Bar | Toggle the status bar on/off. |
| <u>H</u>elp | |
| <u>A</u> bout InPhoHdr | Invoke the About InPhoHdr dialog box. |

Toolbar

The Toolbar is a convenient means of accessing InPhoHdr control operations. It is only a convenience. All Toolbar operations can be accessed through Main Menu entries or pulldown menus. The Toolbar buttons displayed are:



Reset (same as IPS/Reset)
Set IPS data to default values.



Edit (same as IPS/Edit)
Edit IPS system data.



Open
Open file.



Save
Save data to a system file.



Reset (same as IPS/Reset)
Set IPS data to default values.



Edit (same as IPS/Edit)
Edit IPS system data.



Print (same as File/Print)
Print the current InPhoHdr graph..



About (same as Help/About InPhoHdr)
Invoke the About InPhoHdr dialog box.

IV. Warranty

InPhotonics warrants the echelle spectrograph, exclusive of the laser unit*, to be free of defects in materials and workmanship for 12 months following the date of shipment. The warranty is limited to the original purchaser of the Raman systems and is not transferable. The warranty does not extend to any Raman system that has been damaged as a result of accident, neglect, misuse or as a result of service or modification by anyone other than InPhotonics.

During the warranty period, InPhotonics will repair or replace, at our option, any defective parts at no additional charge, provided that the buyer notify InPhotonics of any warranty claim, obtains a return authorization, and ships the equipment prepaid to: InPhotonics, Inc., 111 Downey Street, Norwood, MA 02062.

V. Customer Support

The technical staff at InPhotonics is available for consultation regarding their products. Should there be any problems with the RS2000 spectrometer system, please call InPhotonics between 8:00 – 5:00 pm EST at 781-440-0202.

* The laser system is covered by the original manufacturer's warranty.