LabRAM HR
Software and Hardware

User Guide

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1. SAFETY

1.1 GENERAL SAFETY INSTRUCTIONS

 The LabRAM series equipment must not be operated without prior reading of this document.

The user manual contains important information on how to operate the LabRAM, safely, properly and most efficiently. Observing these instructions helps to avoid danger, to reduce repair costs and downtimes and to increase the reliability and life of the equipment.

Horiba Jobin Yvon equipment is perfectly safe as long as it has been properly installed and is operated according to the instructions which are given in this instruction manual.
The installation of the equipment is to be strictly carried out by personnel delegated by Horiba Jobin Yvon and should not be handled by the end user.

This manual must always be available whenever operating the equipment.

Any person carrying out measurements, whether it is an engineer or an operator, must be aware of the statements enclosed within this manual and apply its contents.
Tasks requiring familiarity with the manual include routine operation including setting up, sample loading, troubleshooting in the course of work.

 Never make any modifications, additions or conversions which might affect safety without the supplier approval. This also applies to the installation and adjustment of safety devices.

In the event of safety relevant modifications or changes in the behaviour of the LabRAM during operation, stop the equipment, and namely the laser source, immediately and report the malfunctioning to a competent authority/person (ex. Horiba Jobin Yvon Service).

1.2 WARNINGS

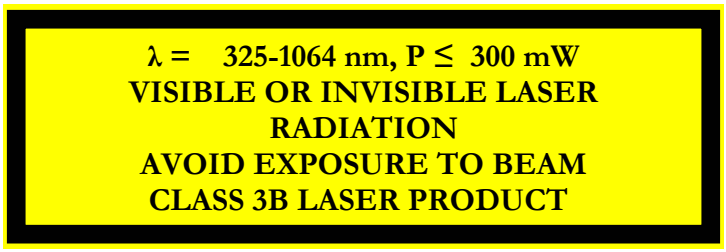
CAUTION: Performance of any procedures not specified by the manufacturer may result a hazardous radiation exposure. This includes removal of covers with laser power ON. There is no user maintenance or service internal to the system with power ON.
When covers or enclosures are removed for any reason extreme care must be taken to prevent the beam being viewed directly by external optics or mirror.
In laser head and power supply, there are high voltages which remain dangerous even if the device is disconnected from the main supply.

The following safety labels are affixed to the system and/or to the optionel parts following different options

Labels 1 to 7 indicate a hazardous situation where there is a risk of serious injury to be caused by laser radiation.

Label 1:

The LABRAM operates with laser sources emitting visible or invisible continuous laser radiation typically bellow 300 mW. The class of the laser product is 3B or 1 with the microscope and external laser sources housings.
DANGER ! AVOID EXPOSURE OF THE LASER BEAM TO THE EYES



Or with the microscope housing
or with external laser and microscope housing.

Label 2:

DANGER ! During operation, the beam laser is emitted in the LABRAM

Location: *On the main cover of the spectrometer and the microscope*

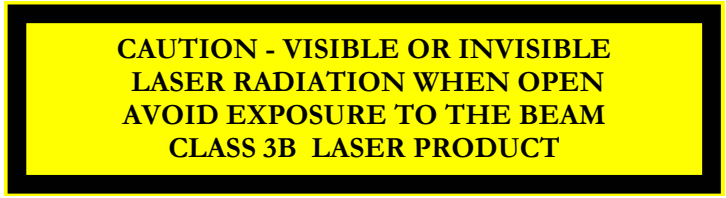
Label 3:

A laser beam is emitted through that aperture.
DANGER ! Avoid exposure to the beam.

Location: *Above the microscope objective*

Label 4:

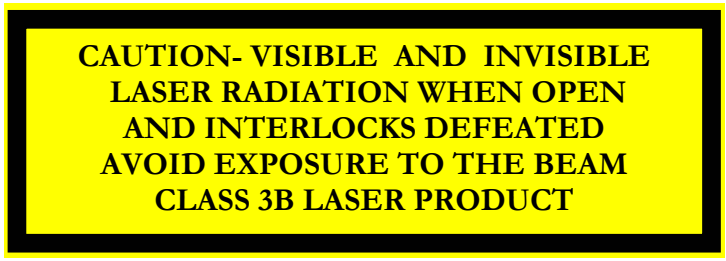
The Labram has a protective cover which is fixed by screws. This cover may not be opened or removed
DANGER ! The laser product class may increase in case of removing that cover and dangerous visible or invisible laser beam may become accessible.



Location: *On the main cover of the spectrometer and the external laser cover for the class 1 version.*

Label 5:

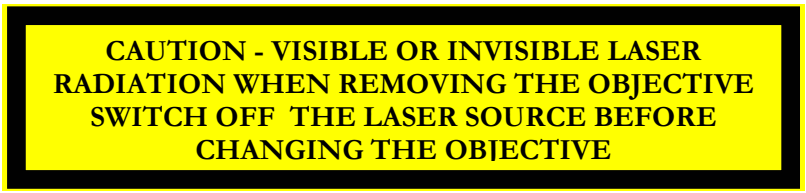
DANGER ! The laser product class may increase in case of removing that cover and dangerous visible or invisible laser beam may become accessible if the covers are removed and the safety switch defeated. FOR SERVICE PURPOSE ONLY



Location : On the microscope cover for the class 1 version and coupling chamber trapdoor.

Label 6:

DANGER ! As microscope objectives are standard components , there are not protected by a safety interlock. **Switch off the laser source before changing the objective.**



Electrical and mechanical Hazard:

Label 7:

Internal laser source label

Location : On the tube of the internal laser source

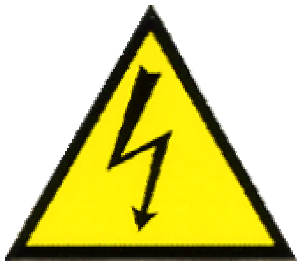
Label 8:

WARNING : Screws has to be removed only for service

Location : On the top ot the main cover.

Label 9 :

DANGER ! Lasers are supplied by high voltage. Always switch off and remove the power supply cord from the main before opening. Take care that all capacitors are correctly discharged.



Location: near the laser connector on the electronic rear panel and the external lasers.

Label 10:

Grounding label

Location : On the rear panel of the main power supply

Label 11:

Protective earth label:

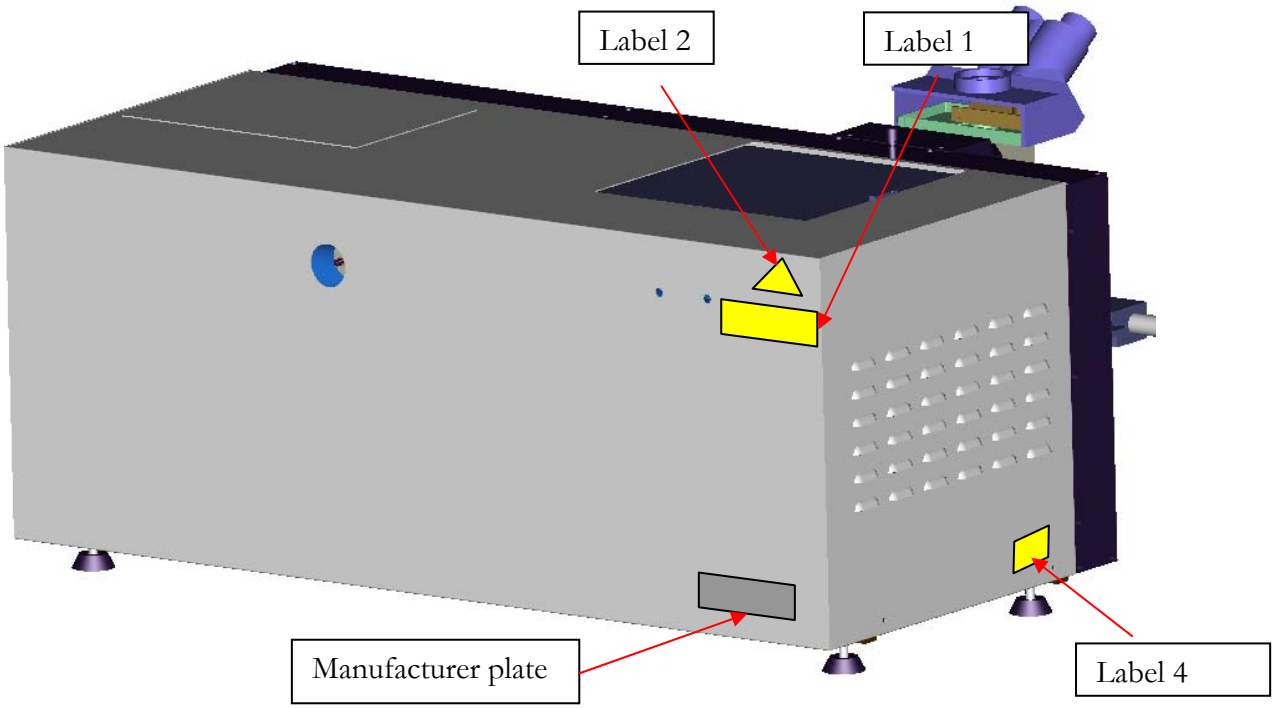
Location : Inside the spectrometer and the main power supply

Label 12:

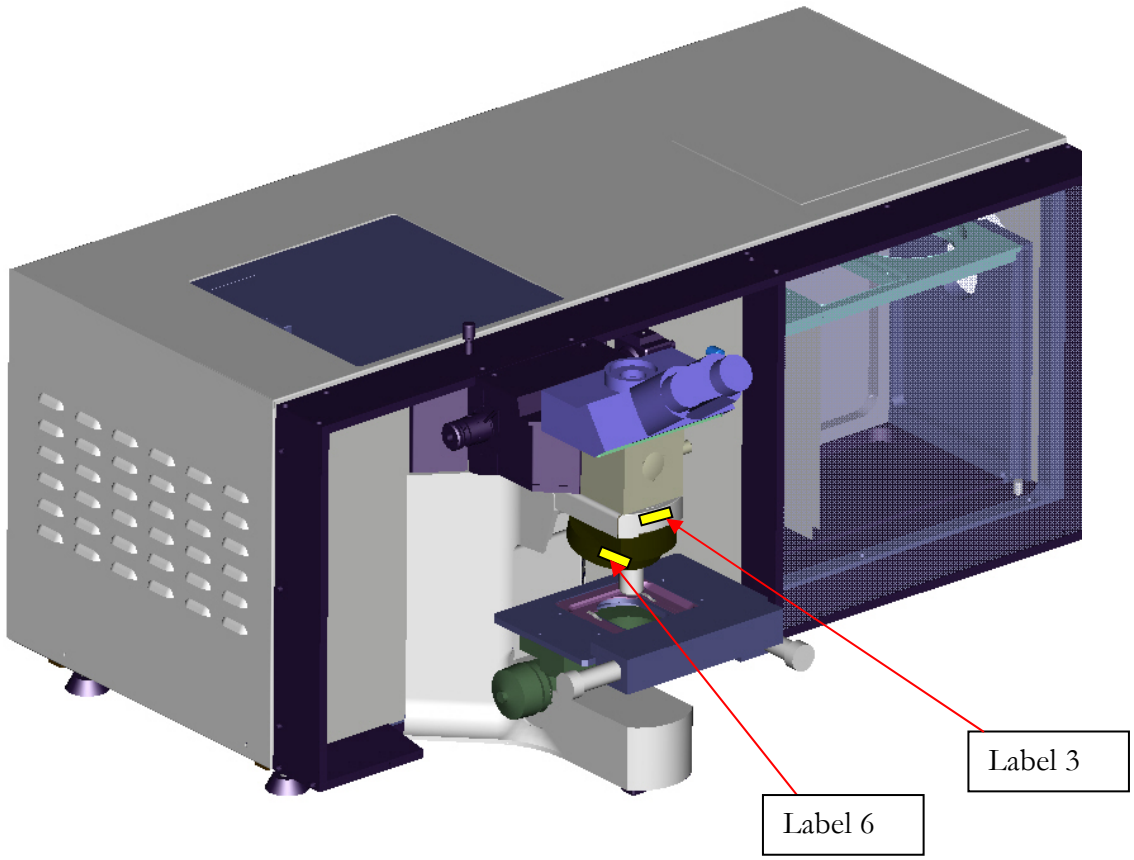
DANGER ! There is a mechanical hazard with the optional motorized table. **Always remove your fingers from the table when motors are in operation.**

Location : on the motorized table.

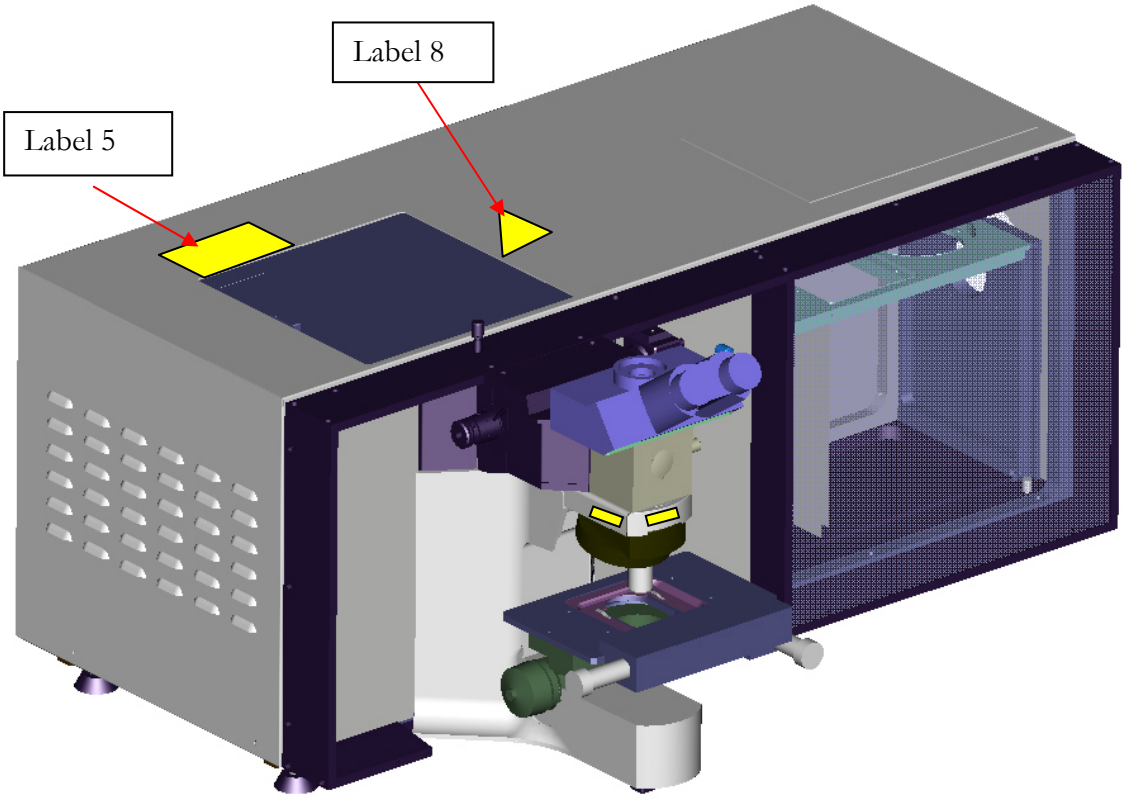
The labels 1, 2 and 4 are affixed on the frame of the LabRAM near the CE stickers.

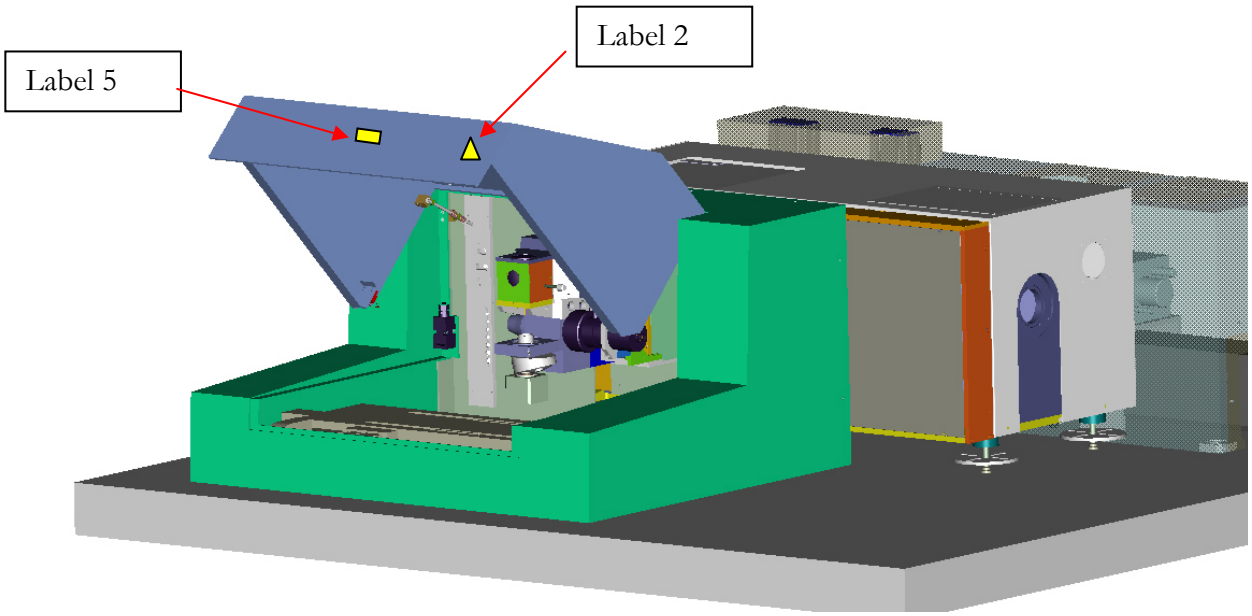


The label 3 and 6 are affixed on the microscope.

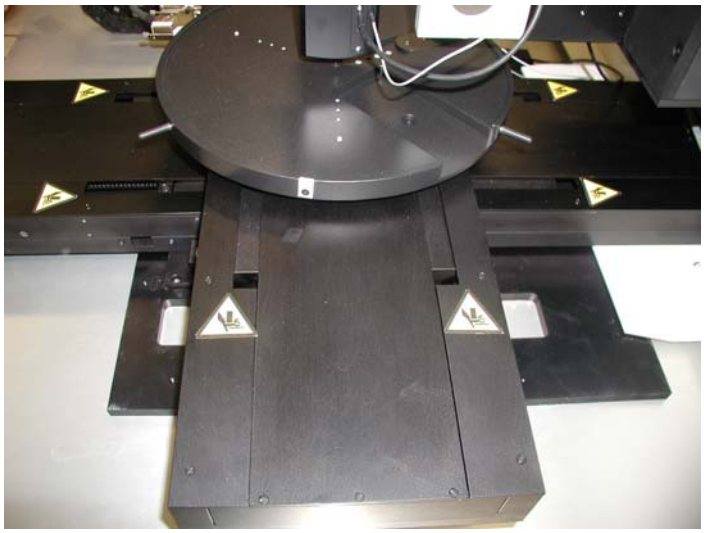


The label 5 is affixed on the microscope enclosure and the slidding panel. These parts are securised by the use of laser safety switches.





The label 12 is affixed on the 300x300 optional motorized XY stage to warn against potential risk of trapping fingers.



The labels 9 and 10 affixed on the rear panel of the power supply

1.3 LASER RADIATION SAFETY

- *On its basic configuration the LABRAM is a class 3B Laser Product. A Class 1 accessory is available for complete housing of the microscope and the external laser source.*
- *The LABRAM is supplied with an internal laser source, eventually one or two external sources. In case of addition of external source, the end-user must ensure that the laser source installation complies with all the legal safety requirements during operation, maintenance and service. For more information refer to § 1.5safety requirements for leser source installation.*
- *Laser sources used with the LABRAM constitutes a hazard to personnel during periods of operating, maintenance and servicing:*

Lasers are high intensity light sources producing visible or invisible light at specific wavelengths. This concentrated energy in a narrow laser beam may cause damage to biological tissues, especially to eyes. To use lasers safely, it is important to understand that laser's required final product safety classification is determined by essentially three elements: the laser's power, wavelength and housing.

Class 3B laser system: Laser beams and reflected beams could be dangerous. Diffused reflected beams in most cases do not present any problem.

Class 4 laser system: Laser beam represents an acute hazard to the skin and eyes from direct and scattered radiation. Fire hazard must be considered.

- The various parts of the LABRAM giving access to the laser beam have been secured by the means of enclosures and tubes from the laser source input to the microscope. These tubes are firmly tightened and prevent any exposure from the operator to any laser radiation. In the optional class 1 version an housing protect all the microscope and another housing encloses the external lasers.
- In case of addition of laser sources, the beam path from the additional laser source to the LABRAM must be secured by the user with an adequate housing (see § 1.5 Safety requirements for laser source installation).
- In class 3B version, the laser beam remains accessible for a functional use below the microscope in the sample area. The end-user must ensure to operate in safe condtions with all the class 3B safety requirements.

The following precautions must be observed:

- Personnel must never look directly into the laser beam and should wear protective eye wear at all times if protective covers are removed while the laser is switched on.
- All personnel in the vicinity of the laser should also be ordered to wear protective eyewear, if protective covers are removed while the laser is switched on. Only qualified and trained personnel should be permitted to operate the laser.
- Precautions must be taken to ensure that there are no reflecting objects in the path of the laser beam, should protective covers be removed and safety devices deactivated. Only beam stops made out of non-flammable materials must be used.
- Warning signs indicating the area in which the laser is enclosed should be clearly displayed.
- Local and national regulations governing the safe use of lasers should be adhered to at all times.
- Ensure that the laser is properly ventilated using a suitable exhaust. Do not connect the exhaust to breathing air systems (i.e. air conditioning or ventilation systems).
- Viewing laser beam with certain optical instruments (eye loupes, magnifiers, binoculars or telescopes) within a distance of 100 mm may pose an eye hazard and must therefore be avoided.
- The sucking air fan located at the rear of the laser must not be blocked at any time
- **Caution**: Use of controls or adjustments or performance of procedures, other than those specified within this manual may result in hazardous radiation exposure.

The laser warning labels affixed to the system according to the safety regulations (see warning chapter) must not be removed.

The laser can only be switched on with the key switch. This prevents inadvertent or unauthorised starting of the laser. It cannot be operated with the key in the OFF position and the key can not be removed in ON position.

If mishandling of the instrument or of the safety devices results nevertheless in direct eye exposure to the laser beam, the exposed operator should consult a doctor or a competent eye testing institution.

- A security switch mounted on the sliding panel on top of the system which automatically activates the blocking of the laser beam, when this panel is opened to intervene in the optical coupling drawer. A screw is used in order to lock this sliding panel. Therefore, the use of a tool is required to open it.
When such an intervention is completed, make sure to firmly screw it again.

Laser Housing

Laser safety devices must not be made inoperative, except for defined checking procedure (laser power and alignment checking) to be carried out by well trained engineers.
The LabRAM could be equipped with a main device that guarantees a class 1 product in terms of laser safety:

-The CDRH enclosure mounted around the sampling area and embedding the microscope. This enclosure contains laser safety interlocks with approved security switches, which induce automated laser blocking when doors are open to access the sample holder.

1.4 MAINTENANCE SAFETY INSTRUCTIONS

Brief operating personnel before beginning special operations and maintenance work and appoint a person to supervise the activities. The End User must ensure that the operators of the system are fully instructed in the safety procedures.

Ensure that the maintenance area is adequately secured. If the LabRAM is completely shut down for maintenance and repair work, it must be secured against inadvertent starting.

In any work concerning the operation, conversion or adjustment of the LabRAM and its safety oriented devices or any work related to maintenance, inspection and repair, always observe the start up and shut down procedures set out in the manual and the information on troubleshooting and maintenance work.

Adhere to the procedures specified in the manual for routine checks and inspection, troubleshooting and laser alignment checking. For the execution of maintenance work, tools and workshop equipment adapted to the task on hand are absolutely indispensable.

Always tighten any screwed connections that have been loosened during maintenance and repair. Any safety devices removed for set up, maintenance and repair purposes must be refitted and checked immediately upon completion of the maintenance and repair work.

Spare parts must comply with the technical requirements specified by the manufacturer. Spare parts from the original equipment manufacturer can be relied upon to do so.

Never modify the software of programmable control systems without informing and getting former consent from the manufacturer.

 In case of changing of objective , it is recommended to switch off the laser source before operating, even if the access of the system have been secured by the means of enclosures equipped with approved security switches or firmly screwed shielding covers.

1.5 SAFETY REQUIREMENTS FOR LASER SOURCE INSTALLATION

All external laser source used by the end user have to follow the regulation CEI 60825-1 (August 2001)
To comply with legal regulations, the following safety requirements need to be respected when installing the laser source:

		Class 3B
1	Protective housing	X
2	Safety Interlock	X
3	Location of control	X
4	Remote control connector	X
5	Key control	X
6	Emission indicator	X
7	Reset	-
8	Certification and identification	X
9	Class warning label	X
10	Service information and training	X
11	Eye protection	X
12	Laser controlled area	X
13	Laser safety officer	X
14	Fire protection	-

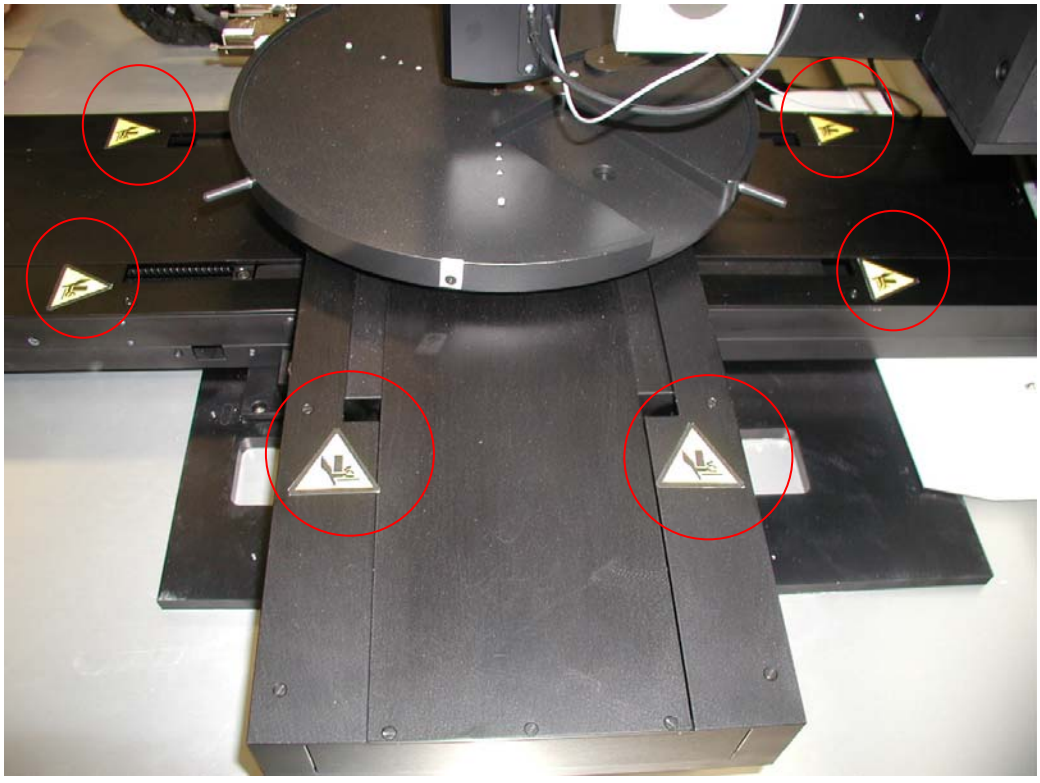
1: The laser beam from the laser source to the LabRAM must be protected by housing.
5: The key must not be removed in “ON” position.
6, 11: Control that the emission indicator is always visible with the eyes wear

1.6 MECHNICAL SAFETY FEATURES

Mechanical safety design provides protection against any hazards which could cause physical injury or burns. Specific mechanical safety features are listed below.

- Exposed corners are smoothened
- Air fans have grill guards with less than 4 mm access. In the event of clogging of the fan grills, these grills should be removed and cleaned/replaced by Horiba Jobin Yvon personnel during maintenance interventions.
- No high temperature components are accessible to touch

Optional XY motorised stage (case of the 300x300 XY stage):
It is highly recommended to take precautions when using this stage. Indeed, this motorised XY stage presents risks of trapping fingers. The picture below shows the location of the dangerous parts of the stage. They are 8 in total (2 in addition at the back of the stage, directly opposite to the front part, which are not visible on that picture).



The highlighted parts can cause serious finger injury.

2- INTRODUCTION TO THE LABRAM HARDWARE

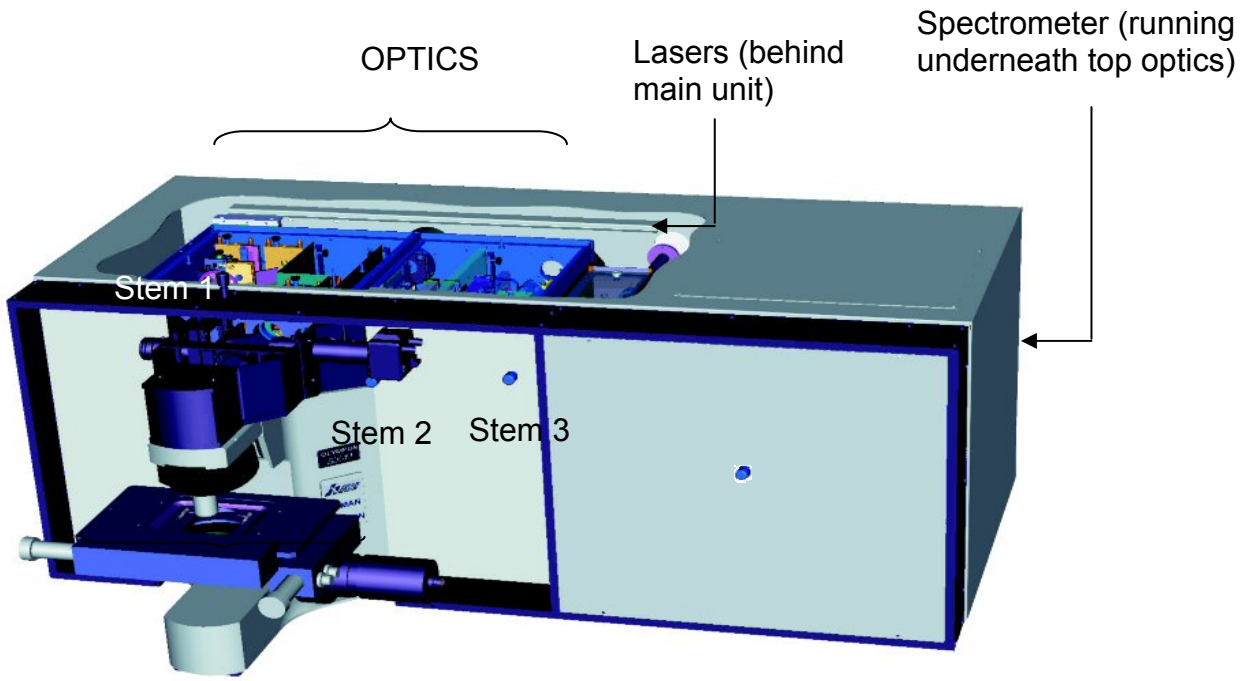
The following diagram of a LabRAM HR system shows the typical layout. The arrangement of stems and accessories is identical for the smaller LabRAM 300 instrument. The instrument can be considered in four parts:

1- Lasers – the HeNe (633nm) laser is internal, whilst other lasers are external, mounted on an extended chassis at the back of the system.

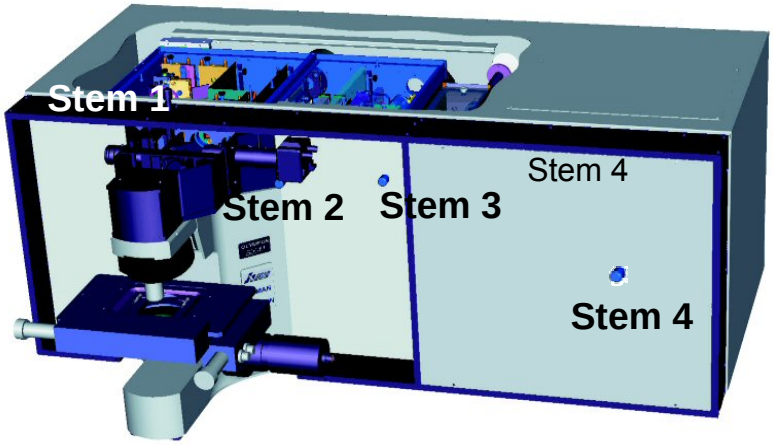
2- Microscope – sampling is carried out through a standard optical microscope.

3- Spectrometer – dispersing the Raman signal into its constituent parts for detection by detector (usually CCD, but other formats can be used).

4- Optics – for coupling the lasers to the sample, and carrying the Raman signal through to the spectrometer.



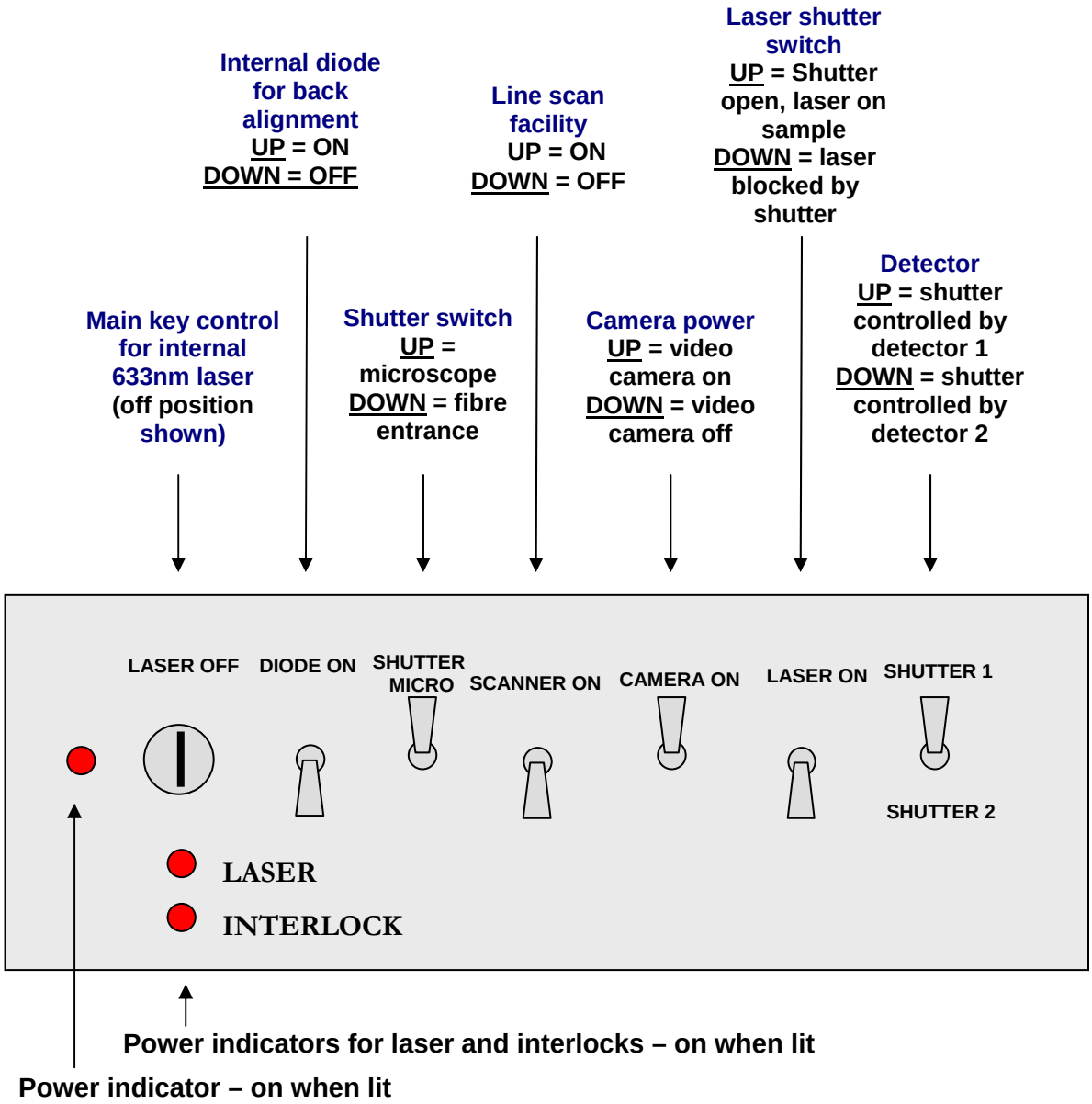
To provide the greatest flexibility and versatility, the LabRAMs include a number of simple stems (or push-pull bars) to allow fast switching between different functionalities.



	Present on LabRam	Present on LabRam HR	Function
Stem 1	√	√	Operates camera beamsplitter. DOWN = camera UP = Raman
Stem 2	○	○	LabRam 300 : operates switching mirror for point mode (IN) and line scan (OUT) LabRamHR : operates switching mirror for vis-NIR (IN) and UV-vis (OUT), or point mode (IN) and line scan (OUT)
Stem 3	○	○	Operates switching mirror for microscope (IN) and fibre entrance (OUT)
Stem 4	√	○	labRam 300 – operates grating turret (in the LabRam HR this is motorised) IN = high resolution (grating 1) OUT = low resolution (grating 2) LabRam HR – operates switching mirror for two detectors. IN = side detector OUT = top detector

√ : always present
○ : sometime present

In conjunction with the software, the LabRAM control box provides an interface between the user and the instrument. An explanation of the switches on the front panel is given below.

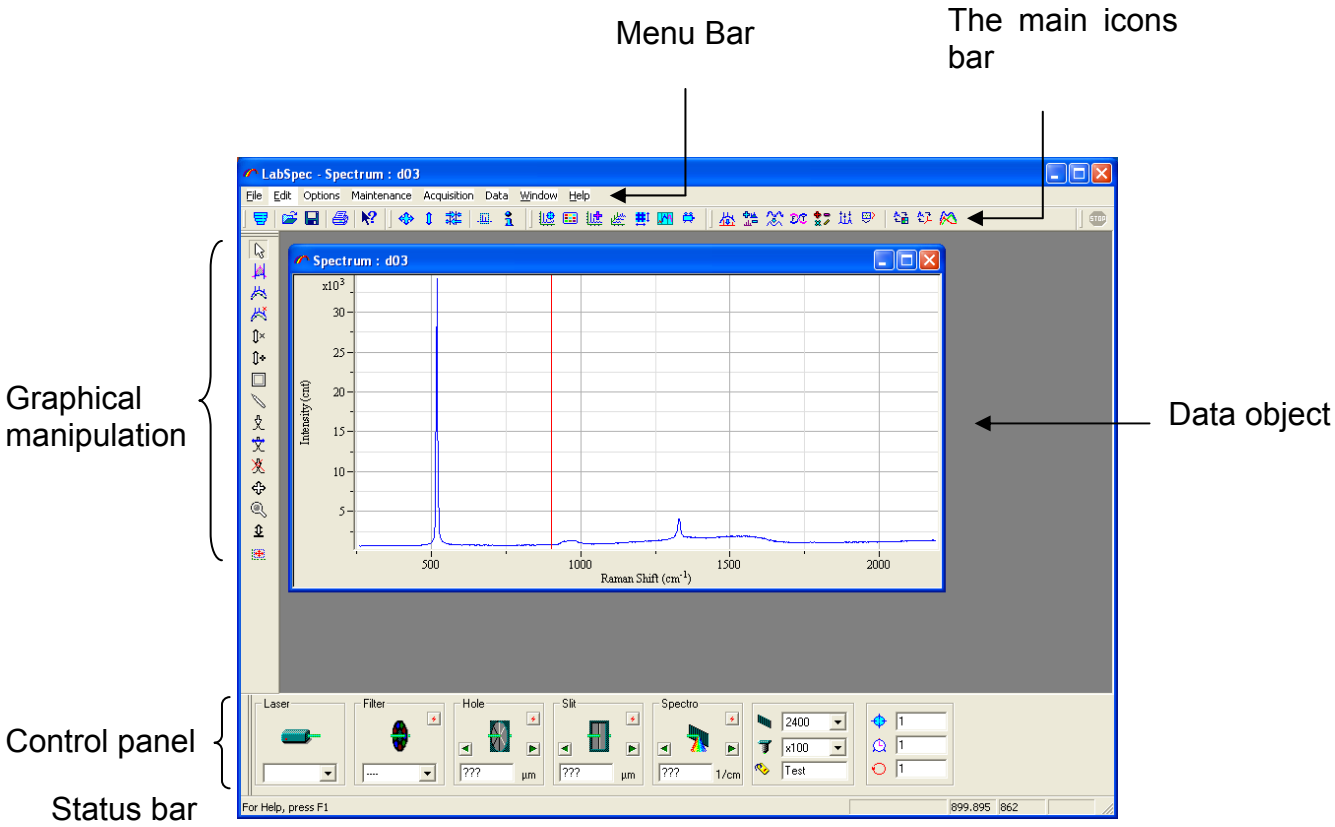


For more information on the hardware, including optical layout, please see the **LabRAM User Manual**.

3- INTRODUCTION TO THE LABSPEC SOFTWARE

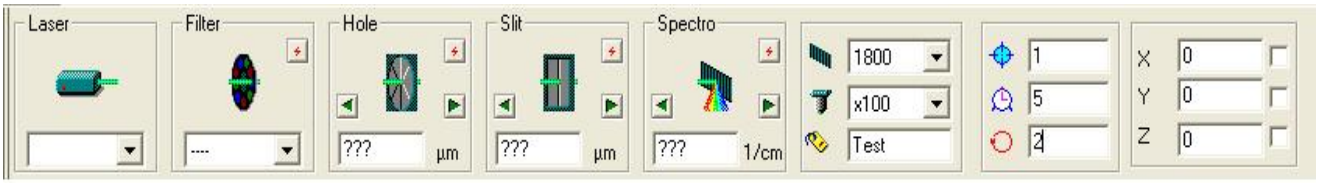
LabSpec 5 is a general data acquisition and data analysis software, based on open NextGen module architecture. LabSpec 5 controls all the HORIBA Jobin Yvon Raman instruments, enables different data acquisition modes (eg. Single spectrum, multidimensional data set, video image etc..)
The data analysis routines include many commonly used Raman and FTIR tools, such as baseline correction, linear and non-linearfilters, peaks fitting Kramers-Kronig transform etc. The mapping techniques enables to generate and visualize map by using different spectral features : band intensity, peak position and so on.
The module architecture allows to customize software to support specific operation, for example read foreign data file format, implement data acquisition trigger etc.
The visual Basic script language of Microsoft is supported, that yield possibility to create macro commands or include specific data analysis function. The LabSpec 5 can be used also as Active X control in third part application.

The Main LabSpec screen can be divided up into a number of regions, as shown below :

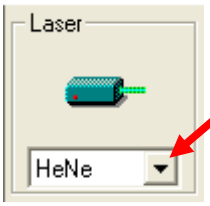


3.1- THE CONTROL PANEL

The Control Panel located on the bottom of the screen contains divisions which are directly related to the System configuration. This panel will show only the devices which are installed on the System. The description below details all of the available sub-units.



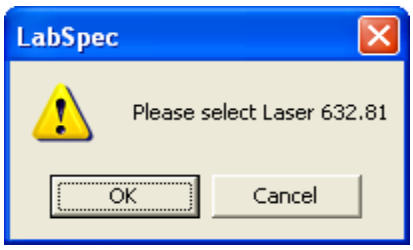
Laser



Select the laser wavelength to be used from a pre-set list.

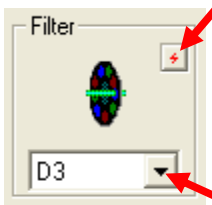
If your instrument is full automated (Aramis instrument) the set of the necessary optical pieces will be automatically set in place so the chosen excitation light reaches the sample.

In case this part is not automated on your instrument a warning message similar to the following on will be displayed.



When everything is in place, click then on the OK button.

Filter



Click here to reset the filter wheel and to set in place the filter displayed in the filter field.

Click here to open the list of the 6 neutral filters installed.

Then select the one you wish to be in place.

Note: The reset function of the filter wheel is useful when for any reason the selected filter is not well in place or does not match the selected one.

There are 6 neutral filters installed with the optical densities 0.3, 0.6, 1, 2, 3 or 4.

[...] = no attenuation (P_0)
[**D0.3**] = P_0 /2
[**D0.6**] = P_0 /4
[**D1**] = P_0 /10
[**D2**] = P_0 /100
[**D3**] = P_0 /1000
[**D4**] = P_0 /10000

Confocal hole

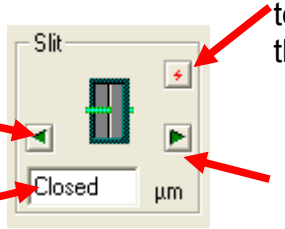
Reinitialise the hole – sends the hole to a known reference point, and then back to the position displayed in the box.

Close the confocal hole.

Type in the value for the confocal hole and press return.

Open the confocal hole to its maximum value.

Slit.



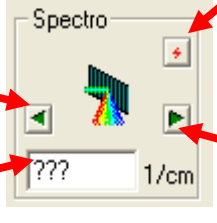
Reinitialise the slit – sends the slit to a known reference point, and then back to the position

Close the slit

Type in the value for the slit and press return.

Open the slit to its maximum value.

Spectro



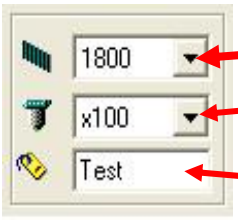
Reinitialise the gratings position– move to the Zero order position, and back to the position displayed in the box.

Send the spectrometer to Zero order.

Type in the central spectral position for the spectrometer and press return

Move the spectrograph grating to the highest value of position.

Options

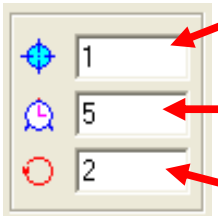


Select grating.

Select microscope objective.

File label – prefix a file name to each accumulated spectrum

Exposure times



Enter here the exposure time value in seconds to be used for the spectrum and image RTD acquisition mode

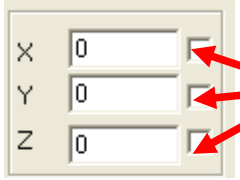
Enter here the exposure time value to be used for the spectrum and spectral image accumulation mode.

Enter here the number of accumulations.

Motorized XY/Z Table

Position of the different axis of the motorized XY/Z table.

Enter here also the position you want the table to be moved.

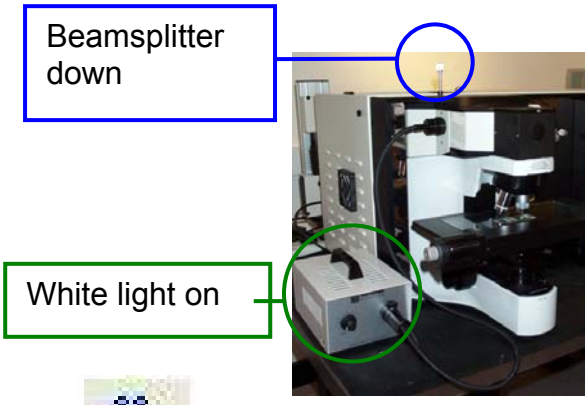


Select the small blank box attached to each table moving axis to have the corresponding position value refreshed in real time even when moving with the joystick.

3.2- WHITE LIGHT ILLUMINATION – IMAGE ACQUISITION

The LabRAM is equipped with standard white light illumination of the sample, by reflection and/or transmission. A colour camera linked to the software allows the sample to be visualised, and the image captured on the computer and saved.

- Put the camera beam splitter into place.
  DOWN = camera
  UP = Raman



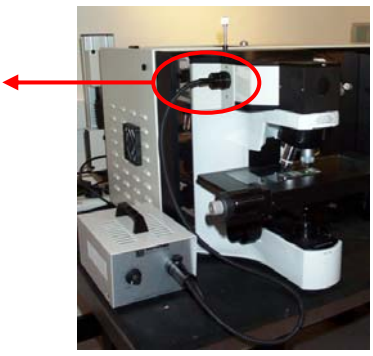
- Turn on the white light illumination.

- In the software, click on the **video** icon to start the camera read out.

- To stop the continuous readout, click on the STOP icon on the top right hand side of the screen.

- Remember to turn off the white light illumination, and take the camera beam splitter out (=UP) before starting a Raman measurement.

To illuminate by transmission only, remove the white light fibre optic from the top left port of the microscope:



4- THE LABSPEC SOFTWARE FOR DATA ACQUISITION

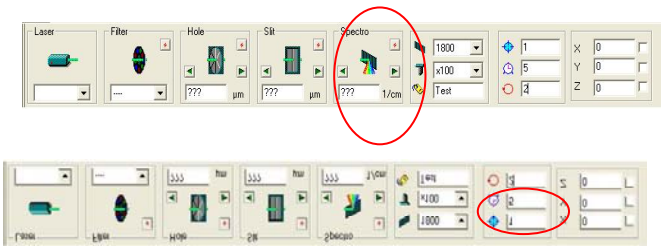
4.1 ACQUIRING A SPECTRUM

The LabSpec software provides the user with a number of methods for acquiring a single spectrum.

Real Time Spectrum Adjustment

This method is primarily designed for a fast display of the spectrum on screen corresponding to a single shot window. The update is continuous, providing a useful way of adjusting the focus position to maximise the Raman signal, and quickly monitoring the stability of the spectrum.
Each spectrum displayed replaces the previously displayed spectrum – there is no averaging or accumulation of the spectra, and no extended coverage possible. To do this you must use **Spectrum Accumulation** (see below).

- Ensure the central spectrograph position has been correctly selected (remember, the position typed into the "spectro." window corresponds to the central position of the resulting spectrum).
- Choose the integration time required



- Click on the **Real Time Spectrum Adjustment** icon.

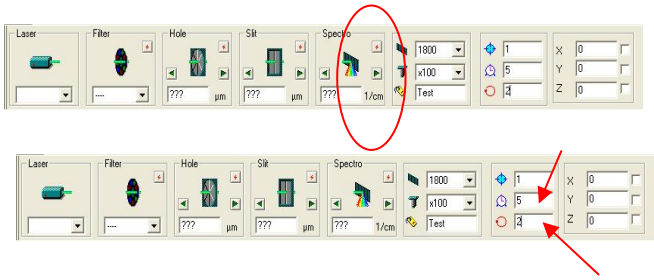
- To stop the continuous readout, click on the STOP icon on the top right hand side of the screen.

Spectrum Accumulation

This method allows spectra to be acquired with multiple accumulations and averaging, and/or with coverage over extended regions.

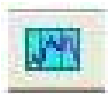
Simple
This method allows a single shot spectrum to be acquired, with user defined integration time and averaging.

- Ensure the central spectrograph position has been correctly selected.
- Choose the integration time required
- Choose the number of accumulations.
- Click on the **Acquisition Options** icon to select a cosmic ray (random spike) removal algorithm. See page 34
- Now click on the Spectrum Accumulation icon to start the acquisition.

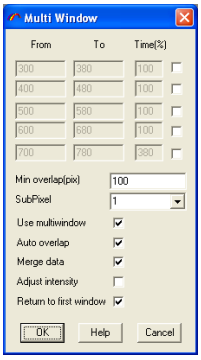


Multiwindow
This method allows a spectrum to be acquired over an extended range, with a defined integration time and averaging. The extended range is covered by taking a number of individual single shot windows and 'gluing' these together. This procedure is fully automated through the software.

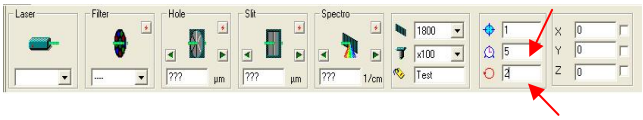
- Click on the **Spectral Windows** icon and choose USE MULTIWINDOW .



- In the SPECTRAL WINDOW PARAMETERS section, type in the Start ("From") and Stop ("To") positions.
- Edit the relative exposure time(in %) of each window. This value is used to compensate the differences of signal level.



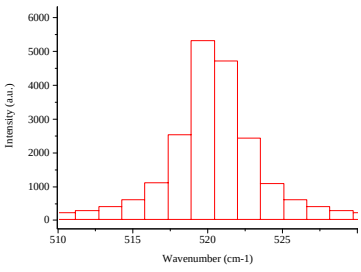
- Select the integration time and number of accumulations from the tool bar at the bottom of the screen.
- Click on the **Acquisition Options** of the main menu to select a cosmic ray (random spike) removal algorithm. See page 34
- Click on the **Spectrum Accumulation** icon to start the acquisition.
- The acquisition can be stopped at any time by clicking on the STOP icon (top right of screen).



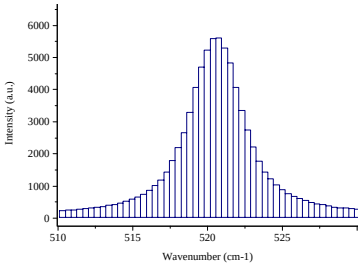
Combining mode

The ***Multi Window*** function allows to set the properties of the acquisition in multi window mode. This mode enables to record data automatically over an extended range with a defined integration time and averaging. The extended range is covered by taking a number of individual single shot windows and 'gluing' these together..
To acces this Dialog select ***Multi Window*** item in the **Acquisition** menu.

From ..... **.....** Edit here the value of the first limit of the spectral window in the
.... current spectral unit. Select the following ☐ to activate the
.... associated spectral window.
To ..... **.....** Edit here the value of the end limit of the spectral window in the
.... current spectral unit. Select the following ☐ to activate the
.... associated spectral window.
Time ..... **.....** Edit the relative exposure time(in %) of this window. This value is
.... used to compensate the differences of signal level.
Min overlap (pix) Define here the overlap between the individual windows in pixels.
..... A value of 50 gives generally good results.
SubPixel ..... Selecting a value >1 allows to restore the fine shape features. The
.... method is based on the shifting of the spectrograph position on a
.... distance less than the detector pixel size. The result is to increase
.... the number of data points defining a band (ie, 2 = twice the
.... number of data points, 3 = three times the number etc). Note that
.... this will increase the total acquisition time, and it is suggested that
.... sub-pixel acquisition is only used over limited ranges



sub-pixel



Use multi window Select this box to activate the multi window acquisition mode

Auto overlap ..... Select this box to automatically define the overlapping size.

Merge data..... Select this box to create one data object for each active spectral window. In the other case a data object is generated for each spectral range corresponding to the spectrograph position.

Adjust intensity Select this box to adapt the intensity to the same values on the overlapping parts. This adaptation is based on the linear shift of the data.

Click on the OK button to validate the settings and to close the window

Click on the Help button to retrieve the information concerning the parameters of this window.

Click on the Cancel button to close the window without validating the change setting

4.2 ACQUIRING MAPPED IMAGES AND PROFILES

Introduction

With suitable accessories on the LabRAM, it is possible to acquire XY mapped images, and line (X or Y), depth (Z), time and temperature profiles.
The principal of these measurements involves acquiring an array (2D or 1D) of spectra, with each spectrum acquired with a particular varied parameter (for example, position, or time).

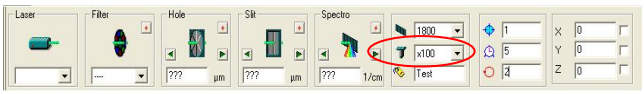
Variation	Description	Hardware requirement
X and Y position	map	motorised XY stage
X or Y position	line profile	motorised XY stage
Z position	depth or Z profile	motorised Z stage/piezo
X, Y and Z position	volume	motorised XY and Z stage/piezo
Time	time profile	no accessory required
Temperature	temperature profile	heating/cooling sample stage

In all cases, the spectral array (3D for volume, 2D for map, 1D for depth, line, time, and temperature profiles) is saved as a single file, allowing fast and easy analysis of the data.

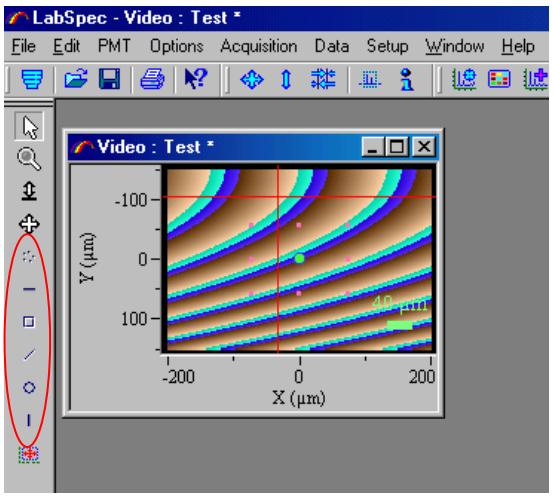
Setting up a mapping/profiling experiment

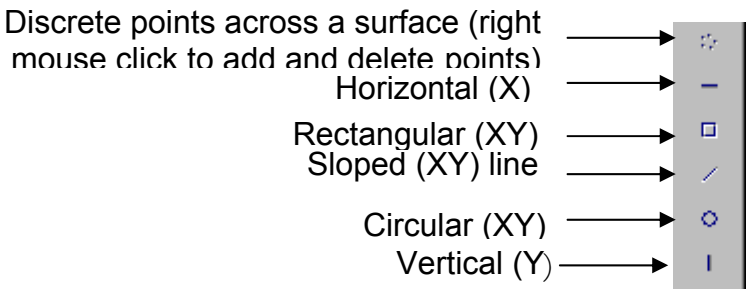
With suitable accessories on the LabRAM, it is possible to acquire XY mapped images, and line (X or Y), depth (Z), time and temperature profiles.

1. On the microscope select the objective to be used for the mapping experiment, and select the *same* objective in the software.



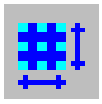
2. If an XY map, XYZ volume, or line profile is to be acquired, obtain a white light image of the sample, and define the area/line to be analysed.

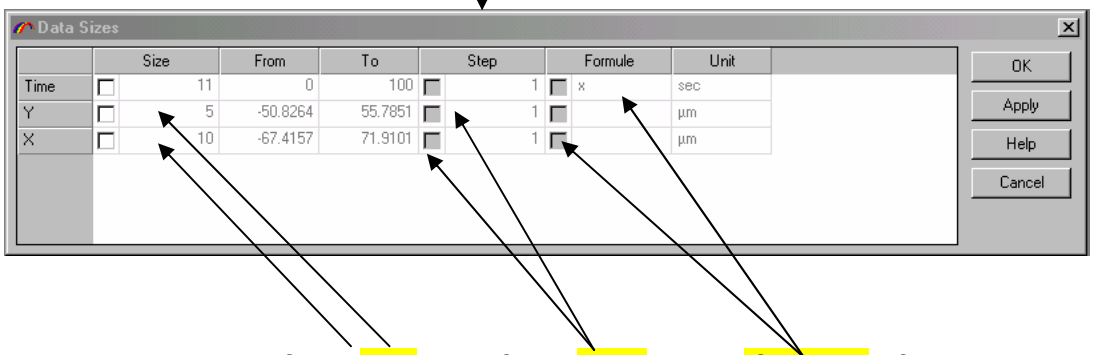




If a depth (Z), time or temperature profile is to be acquired, simply ensure that the sample is correctly positioned beneath the microscope.

3. Click on the Spectral image properties icon in order to define the mapping parameters.





XY map set up by defined size or defined step or by a formula. If size is defined, step will adjust accordingly, and vice versa

Area/Volume mapping

→ X, Y (Z)

For area mapping X and Y dimensions need to be defined. For volume, define the Z dimension as well.

Line profile

→ X (Z)

For horizontal line profile, X dimension is defined only

→ Y (Z)

For vertical line profile, Y dimension is defined only.

→ X Y

For sloped line profile, X and Y dimensions are active, but *size* and *step* are defined only through the X dimension.

Time profile — For time profile, define time only

Depth profile — For depth profile, define depth only

Temperature profile — For temperature profile, define temperature only

Further specific details:

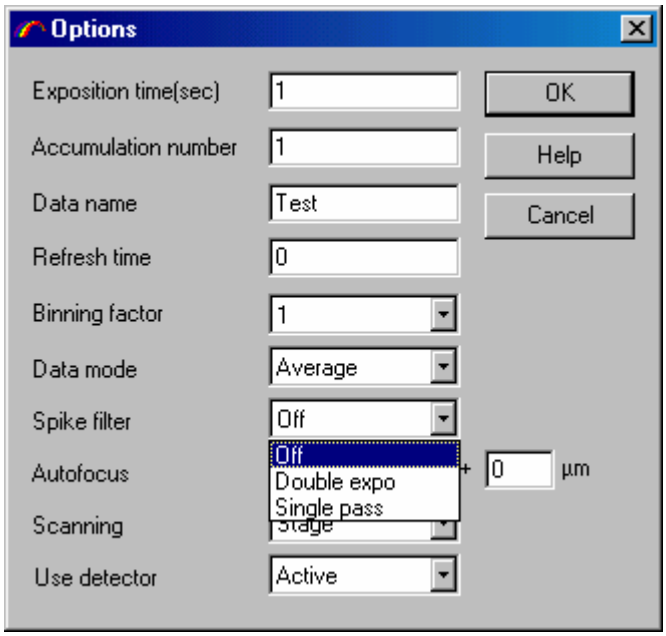
For time profiles, the step size is in seconds, and defines the time between the start of each acquisition. Note that the overall acquisition time per data point must be less than the step size.

For depth (Z) profiles, a negative number in the **variation** box implies moving the analysis point *into* the sample (ie, -20 → 20 µm will move 20 µm below the start position, and step its way up to 20 µm above the start position). The start position is always defined as 0 µm.

4.3- OTHER ACQUISITION FUNCTIONS

4.3.1- Cosmic Ray (Random spike) Removal (via ACQUISITIONS in the menu bar)

The CCD detectors such as those used on the LabRAMs are sensitive to other forms of radiation, and in particular to random events known as 'cosmic rays'. These can interfere with acquisition of spectra by registering as very sharp and strong bands in the spectrum.
Since the occurrence of a cosmic ray is random, it is extremely unlikely that a cosmic ray will occur in exactly the same part of the spectrum in two or more consecutive accumulations. Hence, it is possible to use a simple algorithm to detect random events in a spectrum (as opposed to constant features, such as a Raman peak).
In LabSpec there are two algorithms to choose from.

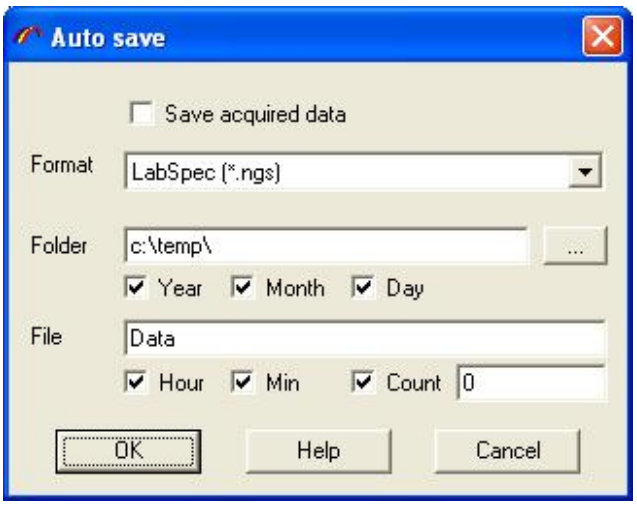


Double expo This is the more robust algorithm, and works by comparing two (or more) accumulations within an acquisition. If a random cosmic ray spike is observed, the spike will be removed. For this algorithm to work, the accumulation number (averaging) must be set to greater than 2.

Single pass This algorithm attempts to locate a spike in a single accumulation acquisition (ie, accumulation number = 1), by analysing bands for sharpness (width) and intensity. This algorithm needs to be used with care, for very sharp Raman bands can easily be modified. However, the algorithm works very well when looking at broad features (such as Raman bands of amorphous materials, photoluminescence etc).
Note that both algorithms can be used for SIMPLE, MULTIWINDOW, single point, mapping, profiling etc.

4.3.2- Auto save (via ACQUISITIONS in the menu bar)

The ***Auto Save*** window allows to modify the properties of the acquisition auto save option.
To access this window select ***Auto Save*** item in the **Acquisition** menu.



Save acquired data.... Select this box to save automatically the data when the acquisition process is finished.

Format Select here the file format. The list of the different format supported is the same one as for **Open/Save** functions.

Folder Edit here the path where to save the files. Click on the  button to select the folder in the tree structure.

Year ..... Select this box to add the year number to the folder name.

Month **.....** Select this box to add the month number to the folder name.

Day **.....** Select this box to add the day number to the folder name.

File **.....** Edit here the file prefix name.

Hour ..... Select this box to add the hour to the file name.

Min ..... Select this box to add the minute to the file name.

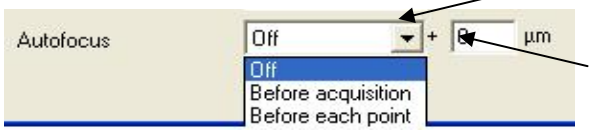
Count ..... Select this box to add the counter value to the file name. The counter is modified each time the auto save function is called. But you can edit the start value of the counter sequence.

4.3.3- Autofocus

The **Autofocus** ensures an optimal focus is reached before an acquisition.

Click on the **Acquisition of the menu bar**. Select Option item of this menu : Check the box to activate the autofocus, and click on the *Autofocus* button to set up the autofocus function.

This allows to adapt or not automatically the Z position to obtain a maximal signal level. The process is based on the detection of the laser beam reflection.



Click on the down arrow icon to display the Autofocus options list

In the + field you can adjust the shift value. Then select if you wish to use or not the Autofocus and at which step of the acquisition process you wish to start the autofocus procedure.

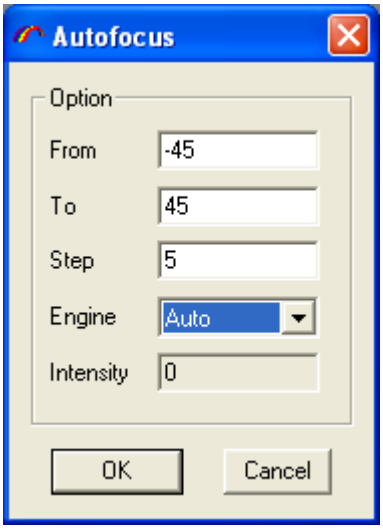
.....* Off **...** The autofocus procedure is not used in the data acquisition
.... process.

.....* **Before acquisition** The autofocus procedure is applied before each data readout

.....* Before each point The autofocus procedure is applied at each new measurement
... point positionning

.....* **Shift value** **...** The shift value allows to adjust the difference between the position where the laser reflection is at maximum level and the one where the spectroscopic signal is at maximum level.

This function allows you to define the properties of the ***Autofocus*** function. To access to this window select **Autofocus** item in the **Acquisition** menu.



From ..... Set the start position (in µm) for the autofocus movement.

To ..... Set the stop position (in µm) for the autofocus movement.

Step ..... Set the step size (in µm) for the autofocus movement.

Engine ... Allows you to select the device used for the autofocusing

- **Auto**: The software select automatically between the Z-motor and the piezo following the size of the movement defined by the From and To parameters.
- **Z-motor**: Force the software to use the Z-motor for autofocussing
- **Piezo**: Force the software to use the piezo for autofocussing.
- **Z-motor & piezo**. The software uses the both devices for autofocusing. A first approach is done with the Z-motor. The research of the final position is then refined by using the piezo.

Intensity. Display the autofocus diode intensity.

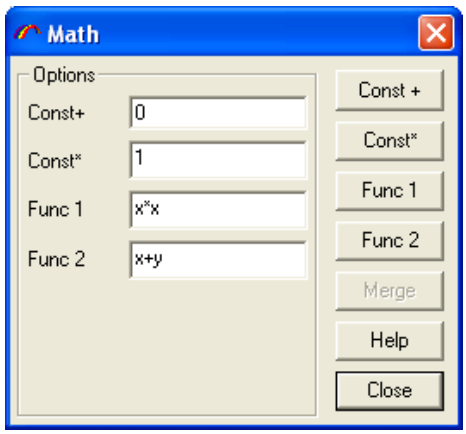
OK. Validate the settings and close the Autofocus window.

Cancel... Close the Autofocus window without validating the setting.

5.1- DATA ANALYSIS FUNCTIONS

5.1.1- Arithmetic 

The **Math Operation** can be used to apply commonly used mathematical formulas to a data object.



✓ **Addition of a constant value**

Enter the value in the **Const+** field and click on the **Const**+ button to add the constant value to the data object.

✓ **Multiplication by a constant value**

Enter the value in the **Const*** field and click on the **Const*** button to multiply the data object by the constant value.

✓ **Application of a complex mathematical function**

Enter the mathematical function in the **Func1** or **Func2** fields and click on the **Func1** or **Func2** button to apply the corresponding function to the data object.
The mathematical formula can include basic mathematical function (+, -, *, /, ^), negating, pow, log, exp, sin, cos, asin, acos, atan, abs, sqrt, step.

For example the “sin(a)” formula replaces the data intensities by sinus function.
The “1000*log(abs(x)+1)” converts intensity to logarithm scale.

The following rules are applied for the variables names:

- the variables **a**, **b**, **c**, … correspond to the values of 1,2, … data axis
- the **x** and **y** value are consider as intensity of data objects.

✓ **Merge function**

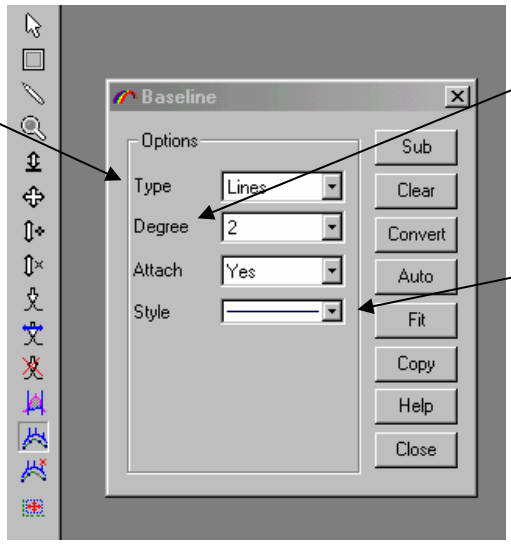
Click on the MERGE button to multiply data objects into a single.

5.1.2- Baseline correction

Allows removal of a background (eg, fluorescence) from a spectrum.

Type of baseline approximation: either *polynomial* (data points lie on a polynomial curve), or line segment (data points joined by straight lines)

Degree of polynomial to be used to approximate baseline



Attachment:
Yes = data points forced to attach themselves to the spectrum,
No = data points can be freely placed anywhere in window.

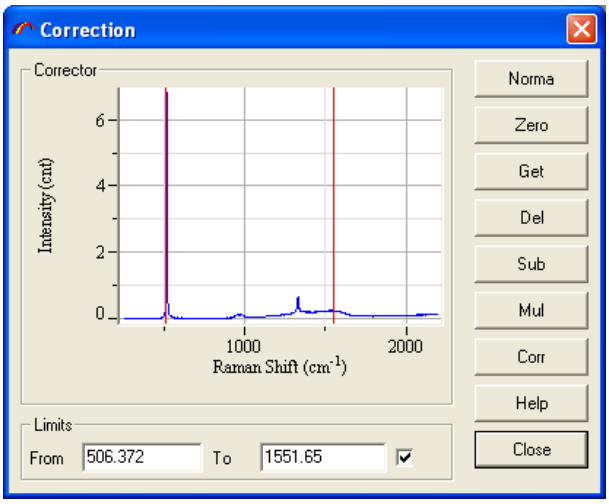
Build the baseline

Erase the points of the baseline

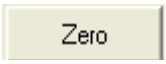
Once the baseline has been correctly approximated, click on *Sub* to subtract the baseline from the spectrum.

5.1.3- Data correction

The **Data correction** function allows you to modify all the traces of a multidimensional data matrix. Some of these operations require an additional spectrum as a second parameter of the operation.

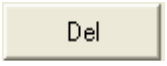


..... The **Norma** button normalizes all the traces to same area value (100).

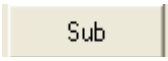


..... The **Zero** button moves all the traces to the minimum intensity level.

..... The **Get** button takes the activated spectrum and put it in **Corrector** frame. This data object will be used as parameter.



..... The **Del** button removes the **Corrector** spectrum.

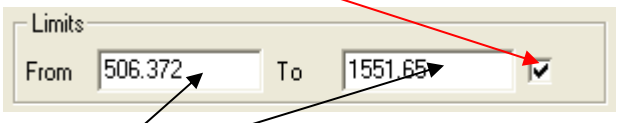


..... The **Sub** button subtracts the **Corrector** spectrum from all the traces.

..... The **Mul** button multiplies all the traces by the **Corrector** spectrum.

..... The **Corr** button subtracts the **Corrector** spectrum from all the traces. The intensity of the **Corrector** is multiplied to fit the intensity of the trace

Limits Select the small blank box if you want that only a part of the trace is used for operation. This parameter is used for **Norma** and **Corr** operation.

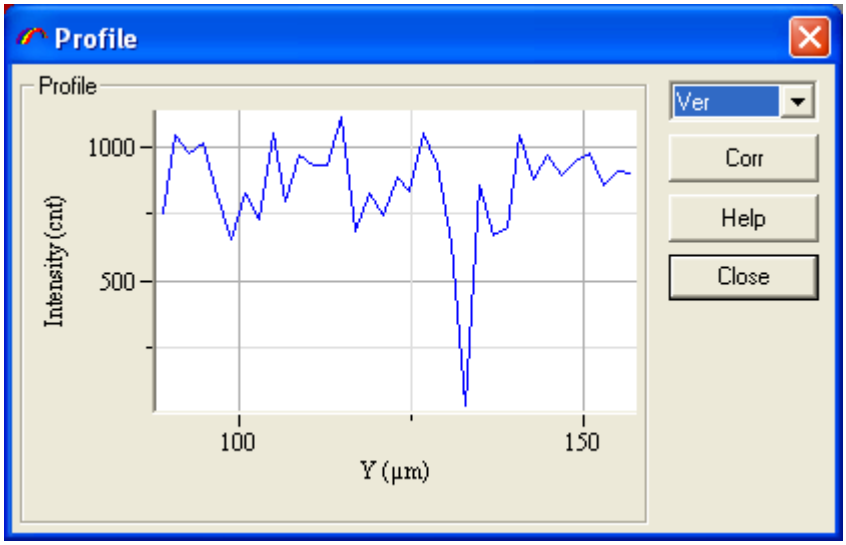


From and **To** Edit these fields to modify the limits of the selected region (linked to the red cursors)

5.1.4- Profile

The **Profile** operation performs a visualization of the vertical or horizontal profile of an image.
To start a **Profile** operation :

- Load an image and activate image display window.
- Select cross line pointer by using window menu **Pointer** item.
- Click on the following icon to open the profile window.



Choose **Hor** or **Ver** control to select between horizontal and vertical profiles.
Click on the **Corr** button to replace the image profile. This operation can be useful when you apply some operations to the profile (for example smoothing) and then you want to set data back to the image.

5.1.5- Filtration

This function allows linear and non-linear smoothing and calculates the derivatives of first and second degrees. The Linear Savitsky-Golay smoothing and derivative computing are based on the convolution approach which performs a least squares fit of polynomial.
The larger is the **Size** value and the lower is the **Degree value** result in a higher smoothing effect.

Degree

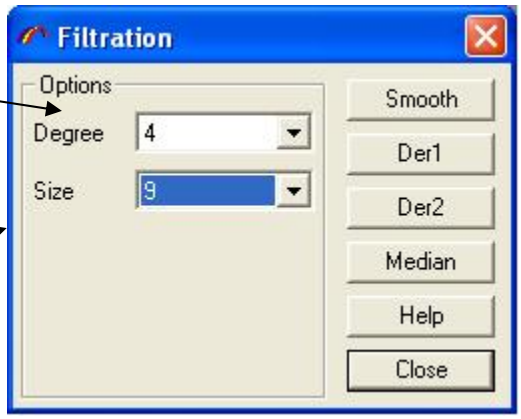
Set in this field the degree of the polynomial.

The lower is the degree the more intense is the smoothing effect.

Size

Set in this field the number of the adjacent data points to be used for the calculation.

The larger is the **Size** value the more intense is the smoothing effect



Smooth ..... Click on the **Smooth** button to perform the Savitsky-Golay smoothing.

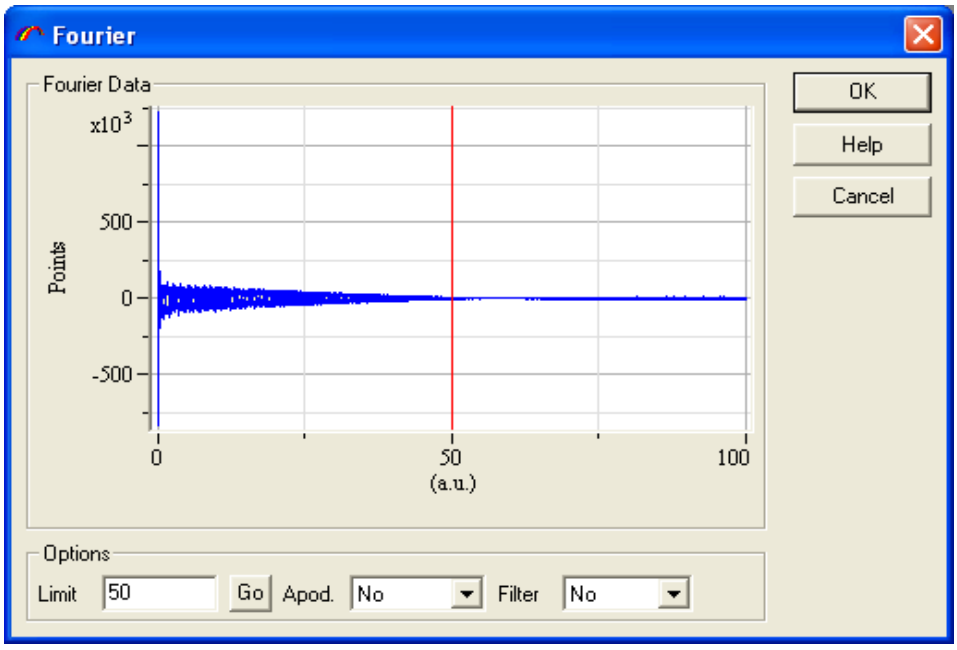
Der1 ..... Click on the **Der 1** button to calculate the first degree derivate.

Der2 ..... Click on the **Der 2** button to calculate the second degree derivate.

Median ..... Click on the **Median** button to apply the median smoothing. The Median smoothing is a non-linear data filter method.

5.1.6- Fourier transformation

The **Fourier Smoothing** is based on the direct Fourier data transformation, applying filter and apodization function and inverse the Fourier transformation. The dialog window shows the real and imaginary Fourier functions and allows you then to select the smoothing property.



Limit – Enter in this field the position of the cut off point in %. This parameter defines the smoothing factor 0 – full smoothed, 100 – no smoothing. Click on the **GO** button to apply the value or drag the pointer to select the **Limit** visually.

Apod – Select here the type of the apodization function with apodization value reaching zero at a **Limit** point.

None	**No apodization function**
Line	**Linear function**
Sqr	**Parabolic function**
Cos	**Cosinus function**

Filter – Select here the type of the filter function.

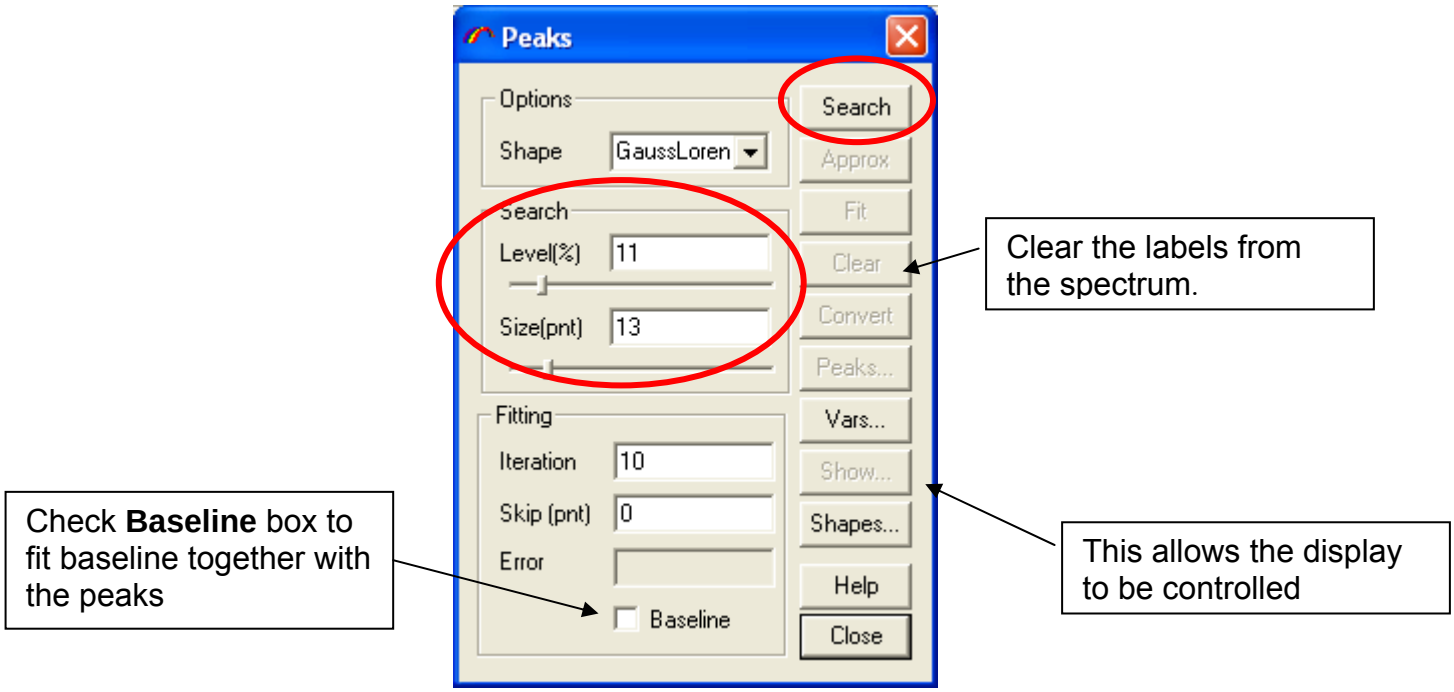
None	**No filter function**
Traffic	**Traffic function**

5.1.7- Peaks and Bands operations

Allows peaks within a spectrum to be quickly labelled, and for particular bands to be fitted in order to accurately calculate band position, width, amplitude and integrated area.

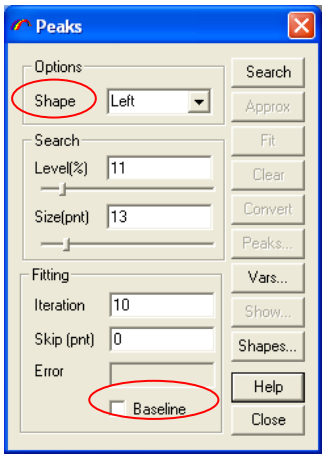
Peak Labelling

To activate the peak labelling algorithm, either click on the *Search* button, or adjust the *Level(%)* and *Size (pnt)* scroll bars. These two scroll bars control parameters used within the searching algorithm for locating peaks in terms of the peak size and proximity to other peaks. Adjusting these scroll bars will allow the labelling to be optimised.



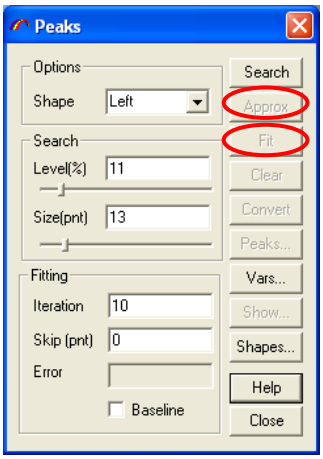
Note : if a spectrum is saved with peak labels, the peak label information will be saved with the spectrum for future reference.

Band Fitting



- Select or edit Peak Shape control to modify the peak curve shape.
- Select the function to be used, and add a baseline if necessary.

- Click on the peak **Label** icon, and mark which peaks are to be fitted.

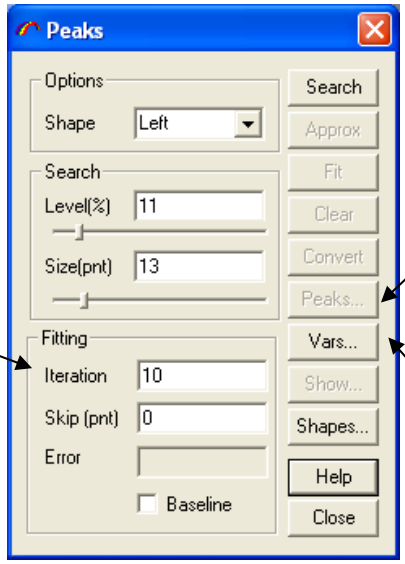


- Once all the peaks have been marked, click on Approx. and then *Fit.*

The results will be displayed on the screen

Note: if a spectrum is saved with the resulting band fit, the information will be saved with the spectrum for future reference.

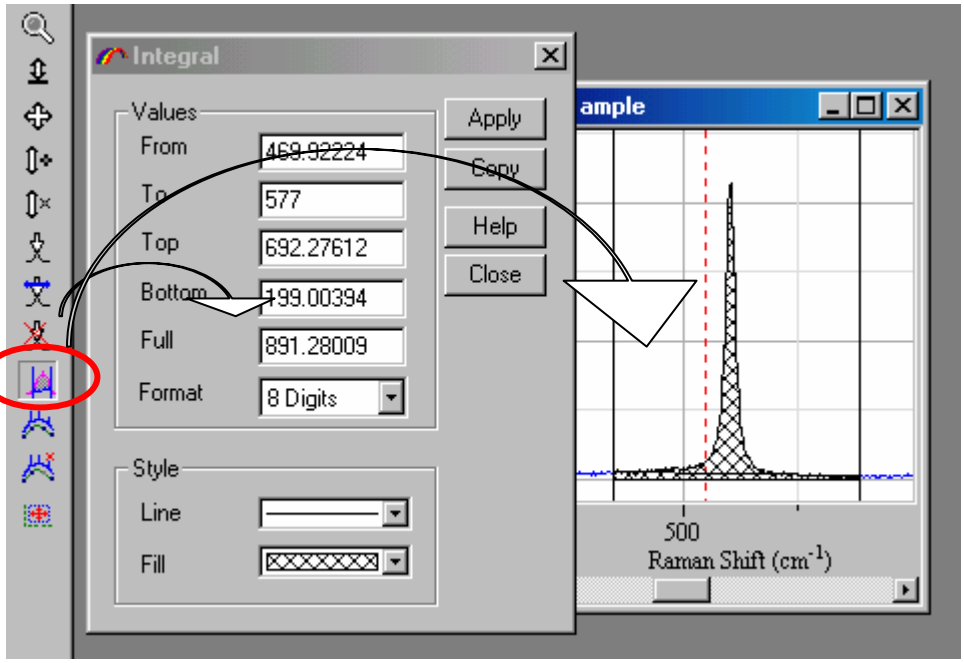
Fit parameters:
Iteration number = number of iterations of the fitting procedure to be completed before stopping.
Skip (pnt) = Increasing the number of skip data point allows to check quickly the convergence of the algorithm and the quality of the initial value selection
Error = displays the error value, as distance between original data and curve sum of all peaks and baselines. This value is named usually as $\chi 2$



Allows initial start parameters to be specified and/or fixed.

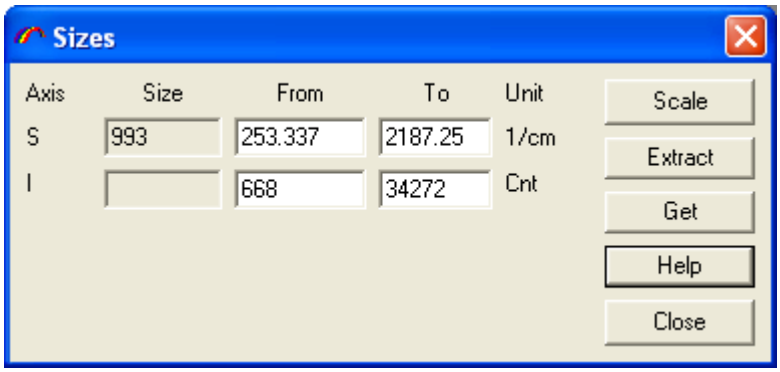
Opens a new window displaying the results of the band fit for baselines and peaks. (p=position, w=full width half max., a=amplitude or max. intensity, g=Gaussian contribution, s=integrated area)

5.1.8- Band Integration



5.1.9- Data size

This function reports the limits for each dimension of the active object in the following window and allows you to re-define it if necessary.
The **Size** field reports the number of the spectral points for the corresponding axis.



..... Click on the Get button to update the limits of the current active displayed object.

..... Use the Scale button to apply the limits to the active displayed object.

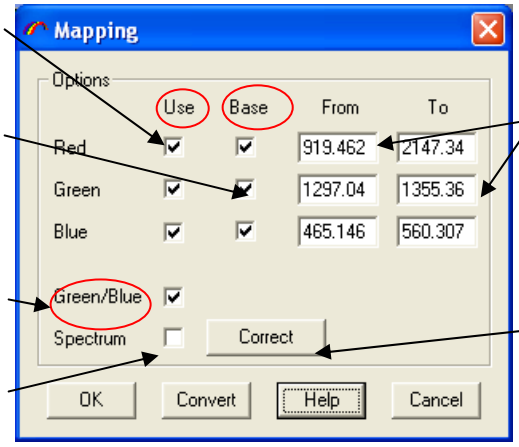
..... Extract the data included in the limits defined in the corresponding fields to build a new object..

5.2- ANALYSING MAPPED IMAGES AND PROFILES

5.2.1- Mapping

The **Mapping** procedure generates a map by using the signal intensity in the selected spectral regions. Up to 4 maps can be displayed when you load or acquire the spectral image: the first three are the average signal intensity and the last is the signal ratio.
The selection of the spectral region is done with the **Red**, **Green** or **Blue** pointer in the spectral image window.

Check **Use** box to generate the corresponding map.
Check **Base** box to subtract baseline.



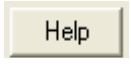
You can edit **From** and **To** fields to adjust the limits of the spectral regions.

Check Green/blue box to generate the map of the corresponding ratio.
Check **Spectrum** box to see the spectrum of the selected data point(s) .

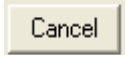
Click on the Correct button to modify data on the selected data point(s).

Click on the OK button to generate the map following the settings and close the mapping window.

Click on the Convert button to convert the current map into spectral image and close the mapping window.



Click on the Help button to retrieve the information concerning the parameters of this window.

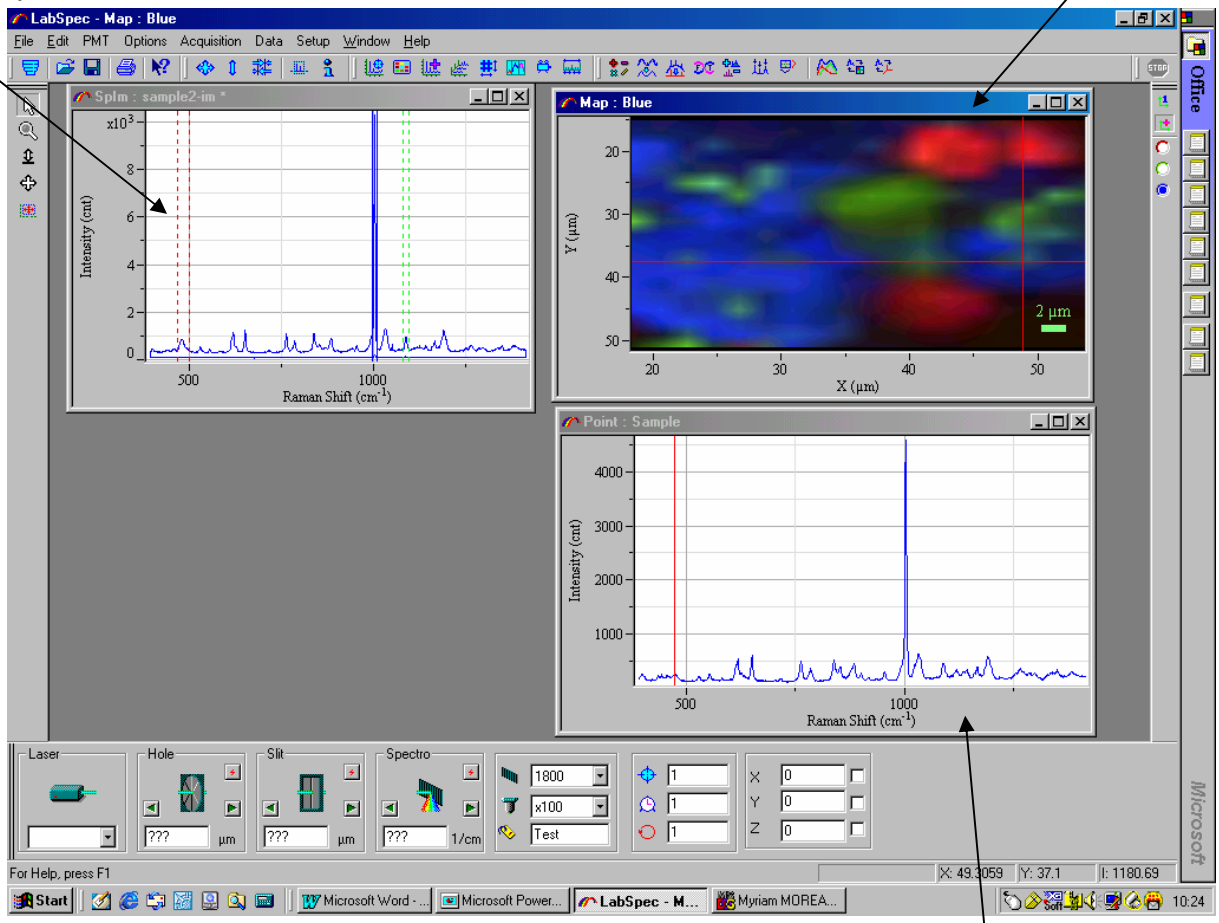


Click on the Cancel button to close the Mapping window without validating the changes setting

Before any analysis is made it is recommended that the data is saved. In all cases, ensure the window containing all the overlapped spectra (**Spectral_Image** or **Spectral_Profile**) is highlighted, and save in the normal way.
A spectral image or profile is initially displayed with three active windows as below:

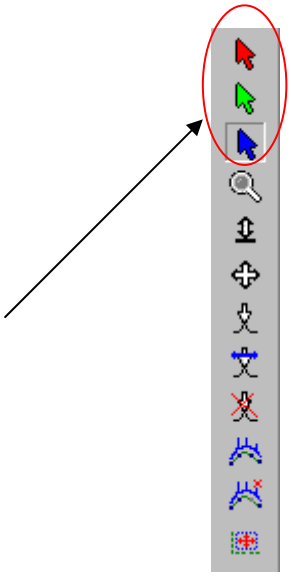
SpIm – containing all data of the image/profile

Map – the resulting Raman image or profile



Spectrum – the spectrum at the current cursor

Note: the following descriptions are based upon analysis of a Raman mapped image, but apply equally to analysis of a line, temperature, time or depth profile.



5.2.2- Analysing with Cursors

The initial method for analysing a mapped image or profile is to use three cursors (**R**, **G** and **B**) to define regions. The image is generated by displaying the spectral intensity between these cursors. For example, in the above diagram, the image can be seen to comprise three coloured regions, which correspond to peak intensities in regions defined by the cursors.
The three cursors are simply selected from the three coloured cursor.
These three cursors appear when the window SpIm is activated. If one or more of the cursors aren't currently displayed on screen, they can be returned by clicking on the **Cursor normalisation** icon  on the toolbar.

Using the cursors provides a fast method of getting useful information from the data. However, in order to distinguish different components this method does require that there are distinct, non-overlapping peaks which can analysed through the cursors.

5.2.3- Analysing with Modelling

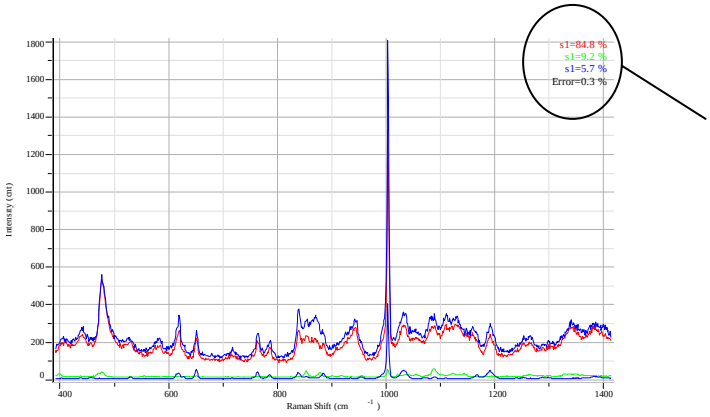
With the modelling functionality, it is possible now to distinguish spectral components that have a large number of overlapping bands, and look at the distribution of any number of species (with the cursors, this is limited to just three – one for each cursor).
The modelling algorithms are based upon correlation fitting of known reference spectra (the models) to the raw data. These model spectra can in fact be obtained separately (ie, run spectra of known raw materials) or taken from the mapping data itself.

- With the map data open, click on the **Model** icon on the toolbar 
-
- If you wish to load in model spectra which you have already acquired separately, open up these spectra.
- Activate the spectrum you wish to use as the first model component.
  If you wish to take this model component directly from the mapping data, use the map cursor to find the spectrum you wish to use, and then activate the raw data spectrum (light blue) in the **Spectrum** window.
- Click on *Get* in the **Model** window.

A new window named **Score** now contains from the models.
If the data is in overlay mode (through FORMAT > Mode in right click scroll-down menu), the image will display all the model intensities overlapped.

The **Spectrum** window now shows not only the raw spectrum at the current cursor position but also information about the correlation fit.
The coloured legends in the top right hand corner indicator the contribution of each component to the correlation fit to provide a match with the raw spectrum.
The coloured spectra displayed comprise:

Light blue = raw data **Red**, **Green**, **Blue** etc = models **Black** = Fit



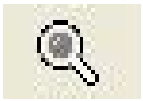
Results of the fit

- A new window will open up which contains the model spectrum.
- This process can now be repeated as desired. Remember, if model spectra are being taken from the map itself, ensure the light blue spectrum in the **Spectrum** window is highlighted before clicking *Get*.

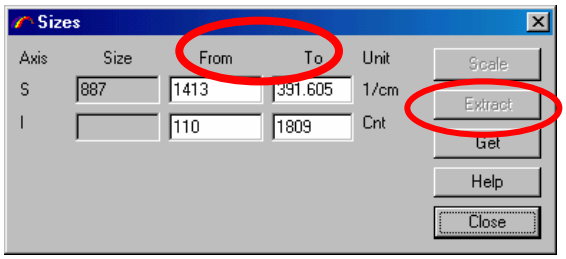
5.2.4- Displaying a map of band position, width, area etc

The data contained within a mapped image or profile can be analysed by a band fitting routine, and the results can then be plotted to give a map showing band position, width, area etc. Such analysis can be of use when investigating changes in phase, stress/strain in materials and other such applications.

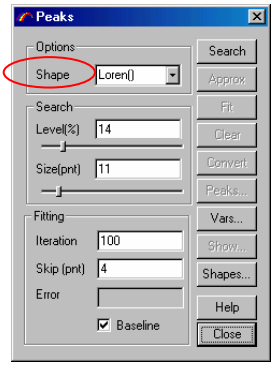
- With the map data open, in the **SpIm** window use the zoom tool to select just the area which contains the bands which are to be fitted.



- Click on the **Data sizes** icon select the limits of the spectral region and then click on the *Extract* button, in order to remove all extraneous data, and leave just the region of interest. It is best that this extracted data is now saved with a different file name, so that the original map with complete data is not lost.



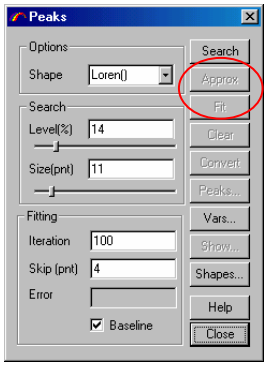
- Open the **Peaks & Bands** window.



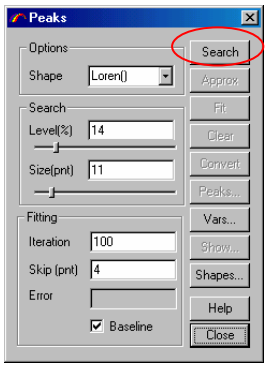
- Choose the band function you wish to use for the fitting procedure, by clicking on the *Shape scroll down menu*. A baseline can also be added at this point.

- With a function selected, now select the peak **Label** tool from the left hand tool bar.

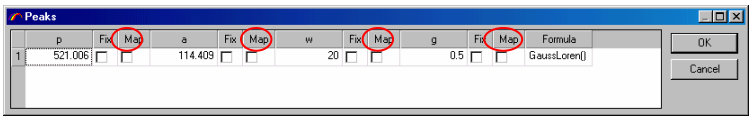
- On the **SpIm** window, mark which peaks you wish to fit.
-
- Click on ***Approx.*** and then ***Fit*** to start the fitting procedure.
  Note: this could take a few minutes to complete for a large map.



- Once the fit is complete, click on ***Peaks.***

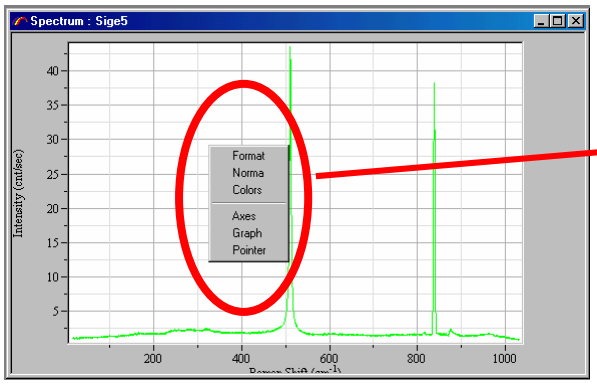


- A new window will open, containing details of the band parameters resulting from the fit.
  These include information on the baseline (if present) and all the bands in the fit procedure. The parameters are as follows:
  p = peak position (cm^{-1})
  a = amplitude (max. intensity)
  w = full width half max (cm^{-1})
  g = gaussian contribution (1=max)
  s = integrated area of band
  The band parameters shown are for the spectrum at the current cursor position.

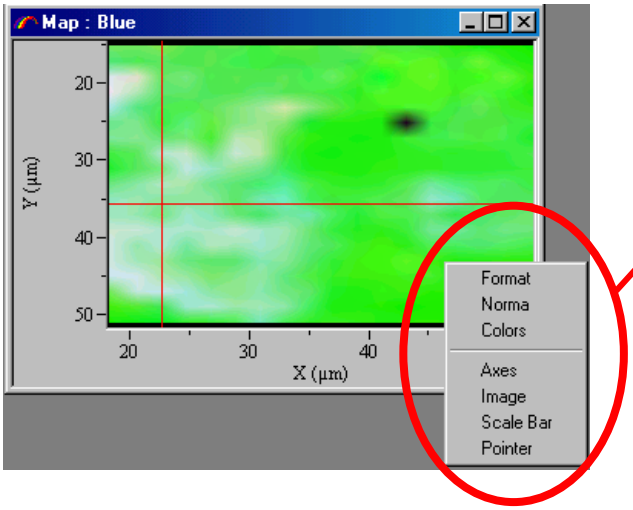


- Clicking on one of the box noticed MAP will generate a new mapped image, giving information about that parameter.
  For example, a map could be generated showing the exact peak position of a band, according to the coloured scale (for example, dark regions → low wavenumber position, bright regions → high wavenumber position).

5.3- DATA DISPLAY FUNCTIONS

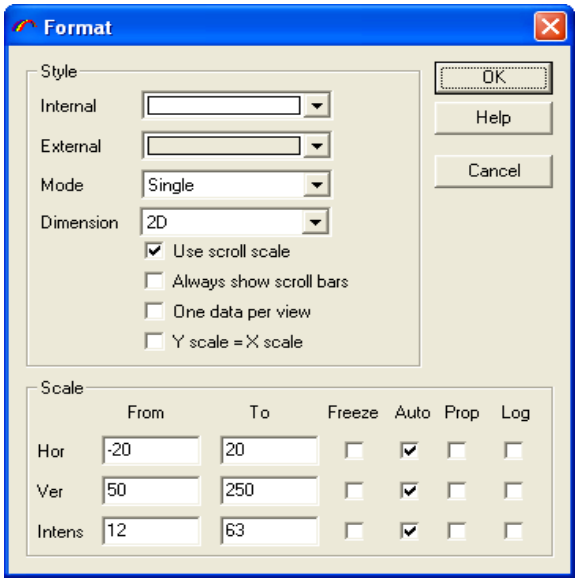


Scroll down menu for spectra display



Scroll down menu for image display

5.3.1- FORMAT



✓ **Internal** **C**lick on this control to modify the color and style of the data field background.

✓ **External** **C**lick on this control to modify the color and style of the window border. Usually it is where the axes are painted.

✓ **Mode** **S**elect one of the following data display modes

Single ... . only activated data object is displayed
Overlay... ..... all data objects are displayed on the same place
Tile ... . data objects will be shown in the separated rectangles
Projection ..... trace of the activated data object will be shown in the separated rectangles
Trace ... . single trace of the activated object will be shown. Use the right scroll bar to change the trace.

✓ **Dimension**
1D / 2D 3D

✓ **Use scroll scale** **C**heck this box to use the window bottom and right scroll bar

✓ **Always show scroll bar** **C**heck this box to always show the scroll bars, when the visual zone is large then the data limits.

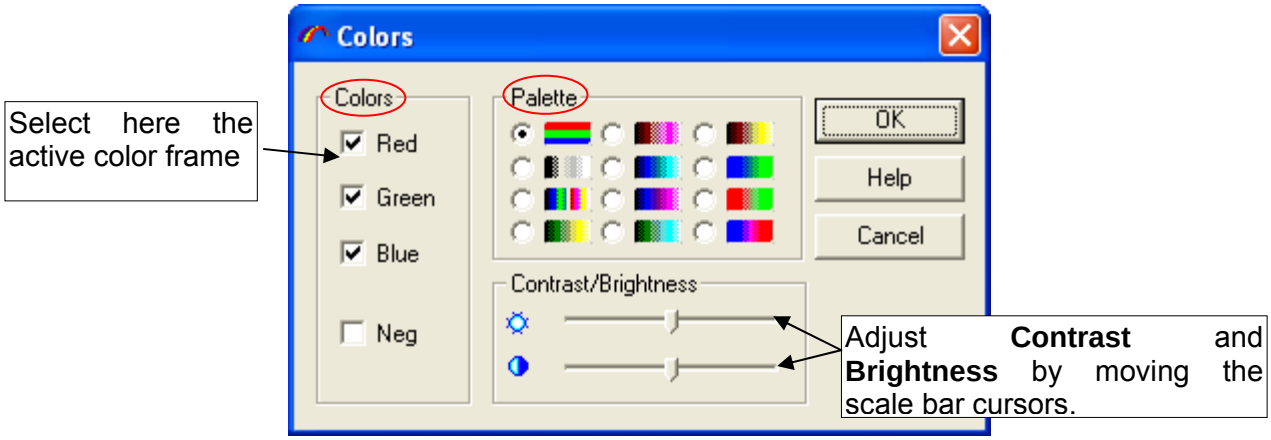
✓ **One data per view** **I**f you check this box, the next time data is displayed a new window will be created.

✓ **Y scale = X scale** **U**ses the same scale for both axes; useful for 2D image presentation.

Scale ..... shows the scale properties for each of the window axes.
From ..... value of low axis limit
To ..... value of high axis limit
Freeze ... fixes axis limits.
The scale will be skipped when normalization function is applied.
Auto ..... enables auto scaling when data object axis is changed
Prop ..... enables proper scale limits for each data object.
Log ..... enables logarithm scale for the axis

5.3.2- Colors

The Colors Dialog enables the image color properties to be modified. Such properties are used when displaying images.
To access this function click on the right mouse button and select **Colors** menu items.



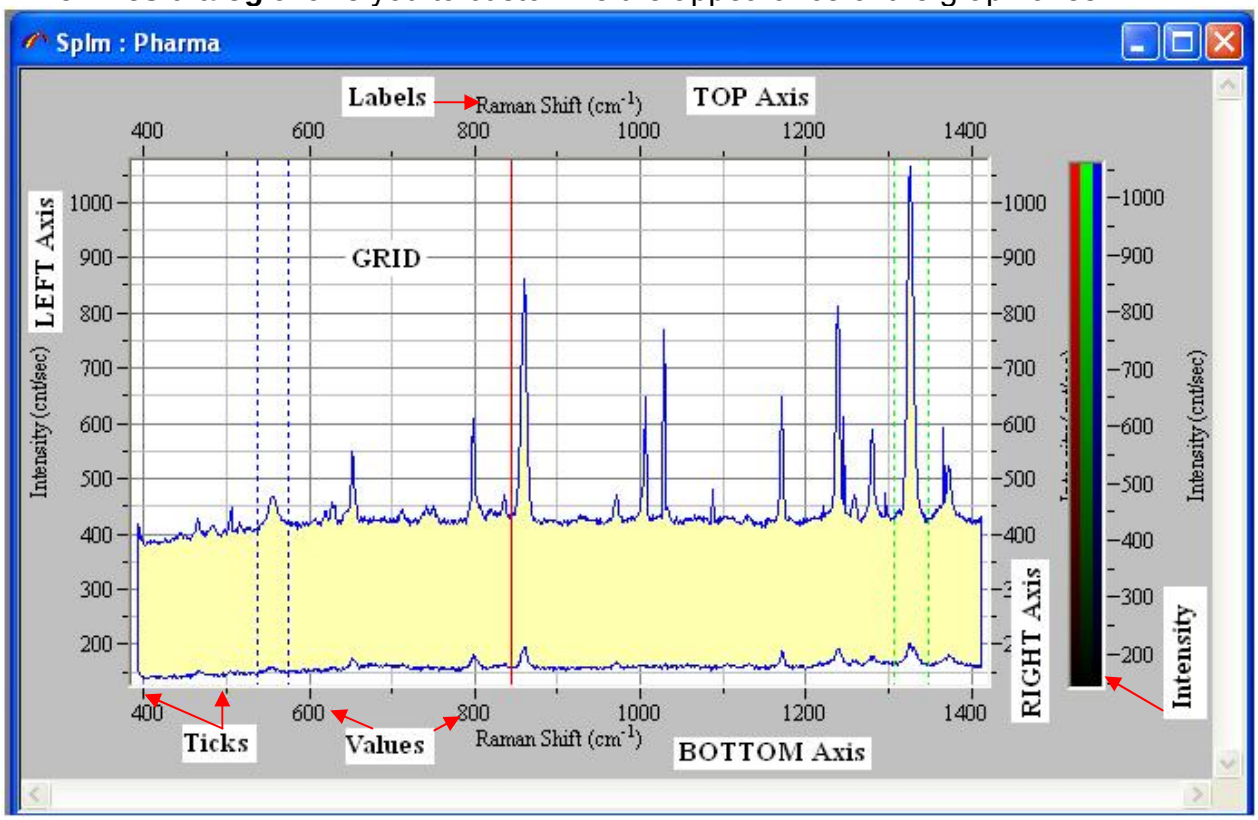
In the **Colors** frame you can turn on/off **Red**, **Green** or **Blue** color.
To make image negative choose **Neg** check box.

In the **Palette** frame select one of the following styles:

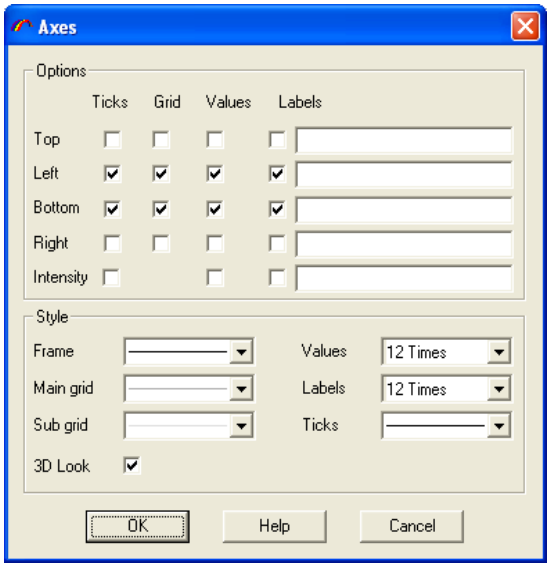
True color. ..... All colors are displayed without modification
Black and White.
False color.
Green .....Yellow scale.
Red .....Magenta scale.
Blue .....Cyan scale.
Blue .....Magenta scale.
Green .....Cyan scale.
Red .....Yellow scale.
Blue .....Green scale
Red .....Green scale.
Blue .....Red scale.

5.3.3- Axes

The **Axes dialog** allows you to customize the appearance of the graph axes.



As shown on the picture above there are 4 axes. The Axes Dialog allows you to define independently each component of each axis. You access to the Axes Dialog by selecting the **Axes** item of the window context menu.



✓ **Options**

Tick ... Check the box to enable the painting of ticks.

Grid .... Check the box to create a grid for tick levels.

Values Check the box to enable the painting of number values associated to ticks.

Labels Check the box to create an axis label and enable customization of the axis label.In the Labels blank field enter the text you wish to be appeared for the corresponding axis.

✓ **Style**

Frame ... click on the control to modify the color and style of axis edge. This parameter is used for a non 3D look.
Main Grid .click on the control to modify the color and style of the main grid
Sub Grid click on the control to modify the color and style of the sub grid
Values ... click on the control to modify the values font.
Labels ... click on the control to modify the labels font
Ticks ... click on the control to modify the color and style of the ticks.
3D Look . check this box to enable a 3D outlook for the edge

5.3.4- GRAPH

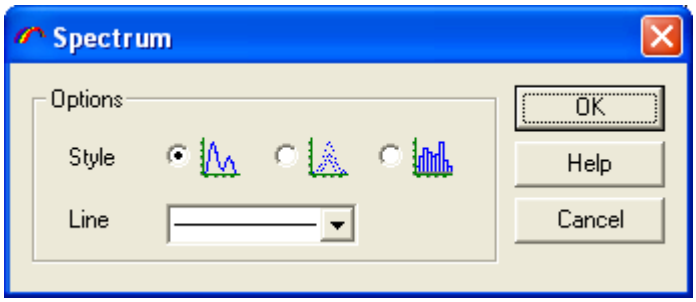
This function allows you to customize the appearance of 1D dimension displayed data objects.(Spectrum or Spectral Image)

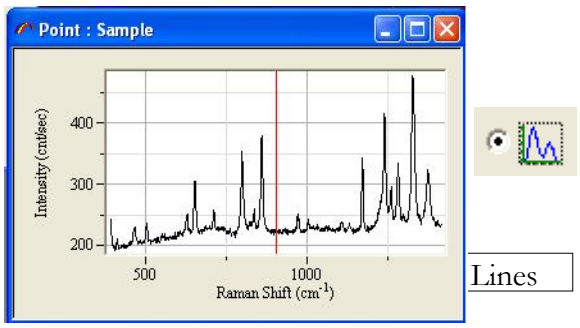
5.3.5- Spectrum

If the active object is a spectrum selecting **Graph** item of the window context menu opens the **spectrum Properties** dialog which allows you to modify the display properties of the spectrum.

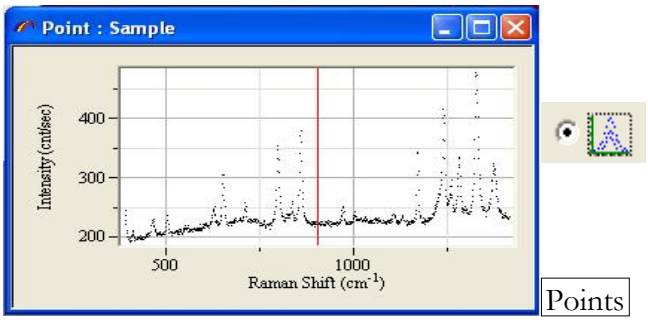
✓ Select one of the **Style** controls to display spectrum as a set of **Lines, Points** or **Bars**.

✓ Click **Line** control to modify the color, thickness and line type.

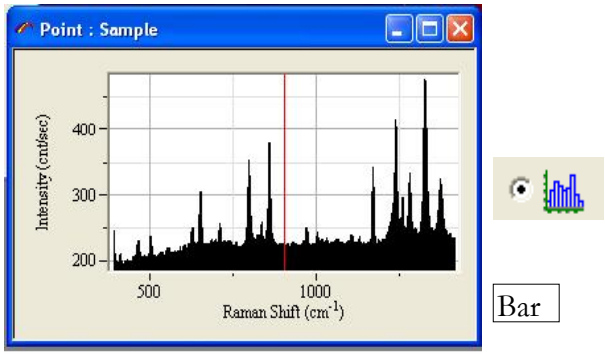




Lines



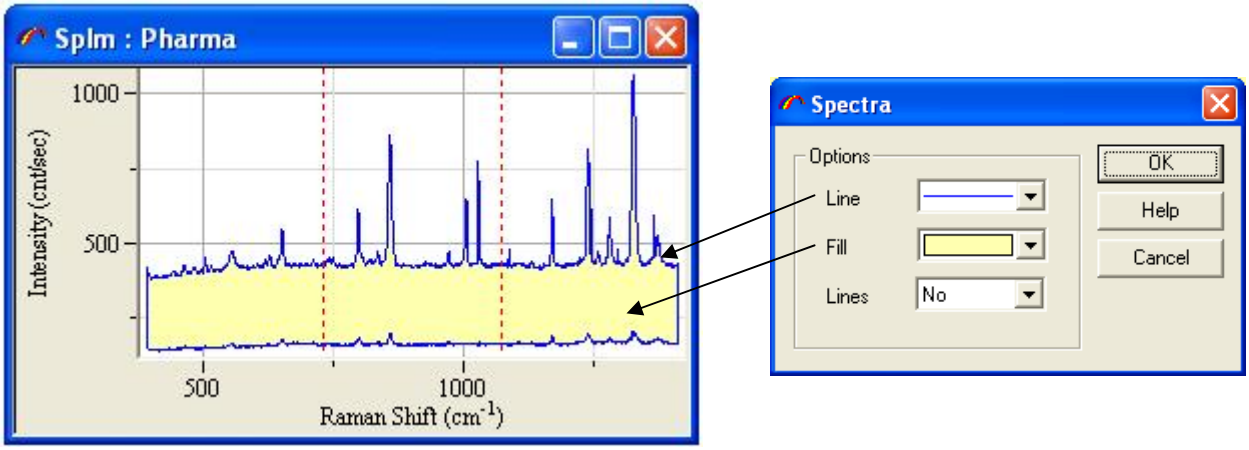
Points



Bar

5.3.6- Spectra

If the active object is a spectral image selecting **Graph** item of the window context menu opens the **spectra Properties** dialog which allows you to modify the display properties of the SpIm object.

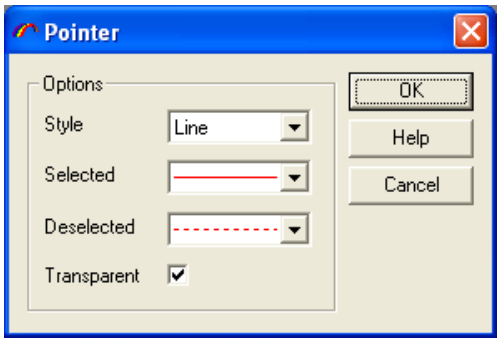


- ✓ Click **Line** control to modify the color, thickness and line type.
- ✓ Click **Fill** control to modify the color and fill style of the filled zone.
- ✓ Click **Lines** control to select the representation mode of all the spectra. You can select to display **All** the spectra , leave the software to display **auto**matically the necessary spectra so it is readable, or as shown on the picture above not to display all the spectra.

5.3.6- Pointers

The **Pointers dialog** allows you to customize the appearance of the pointers. You access it by selecting the **Pointers** item of the window context menu.

- ✓ Click on the **Style** control to choose one of the following pointer types:

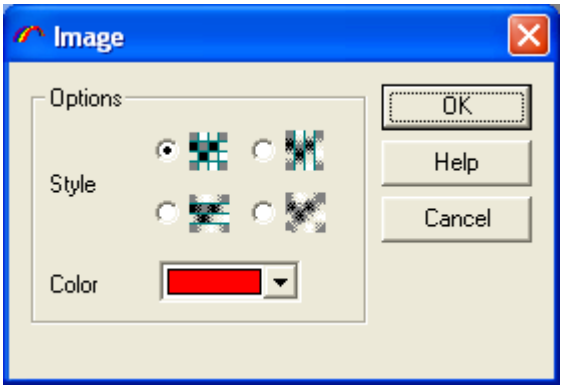


Line ...single vertical line.
Cross .vertical and horizontal lines.
Level ..vertical and horizontal lines.
The position of horizontal line corresponds to the data intensity value.
Double two vertical lines.
Rect ...rectangle.

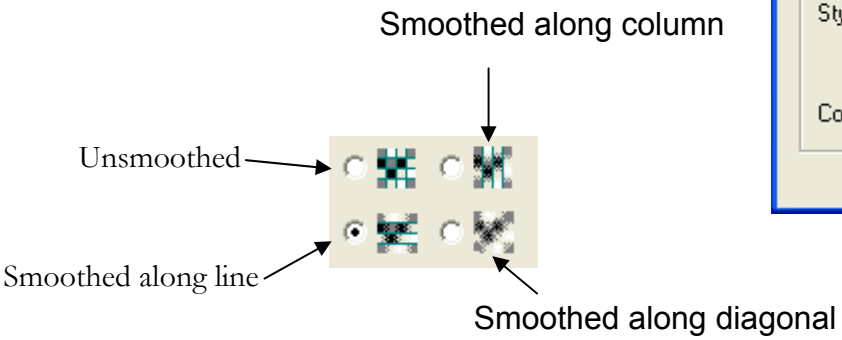
- ✓ Click on the **Active** control to choose the line style, when the pointer is selected (you can drag pointer with the mouse).
- ✓ Click on the **Hidden** control to choose the line style, when the pointer is deactivated.
- ✓ Check **Transparent** box to draw a pointer in transparent style. In such cases the image of the pointer is superposed with the window background.

5.3.7- Image

The **Image Properties** Dialog enables to modify the appearance of the images data objects. To access this dialog, select **Image** item from the window context menu.



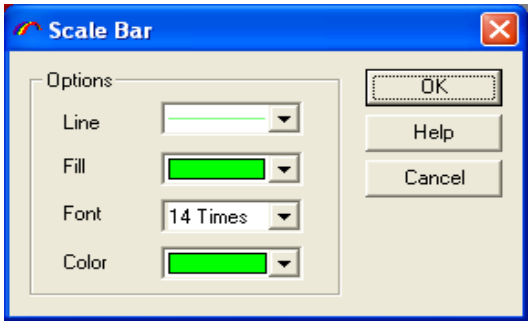
✓ Select **Style** mode, to make or not a linear interpolation of image intensity along X and/or Y axes.



✓ Click **Color** to modify the image color. This color will be used, when you select overlay mode for the data display.

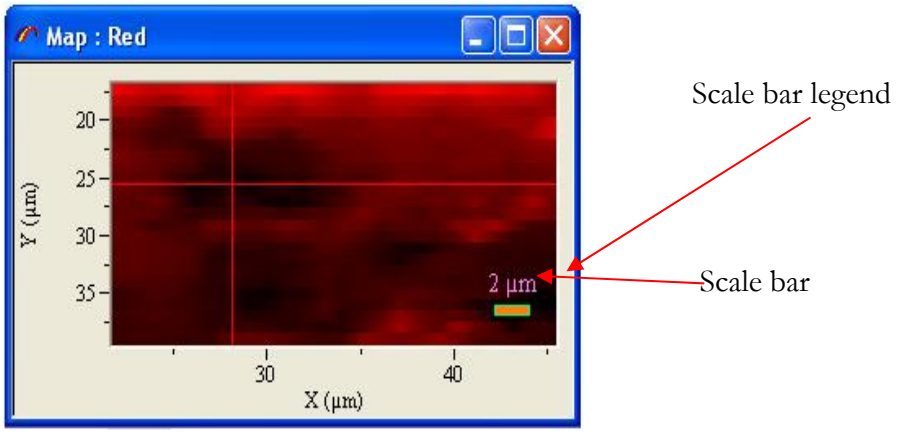
5.3.8- Scale bar

The **Scale Bar Properties** dialog allows you to modify the display properties of the scale bar and its associated legend of the 2D presentations. To access this dialog, select **Scale Bar** item from the window context menu.

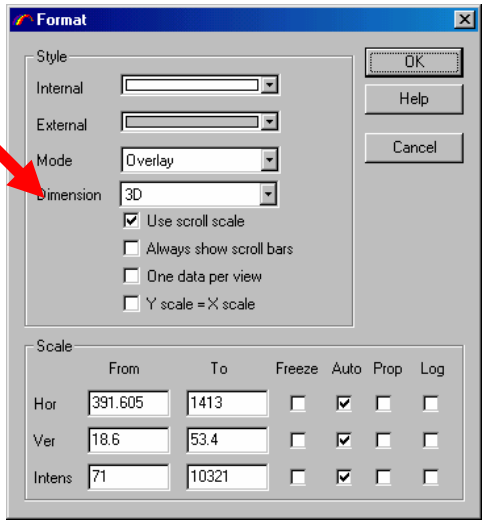


✓ Click on **Line** control to select the bar border style and color of the scale bar.
✓ Click on **Fill** control to select the sacle bar filling style and color.

✓ Click on **Font** control to select they the scale bar legend font properties
✓ Click on **Color** control to select scale bar legend text color.

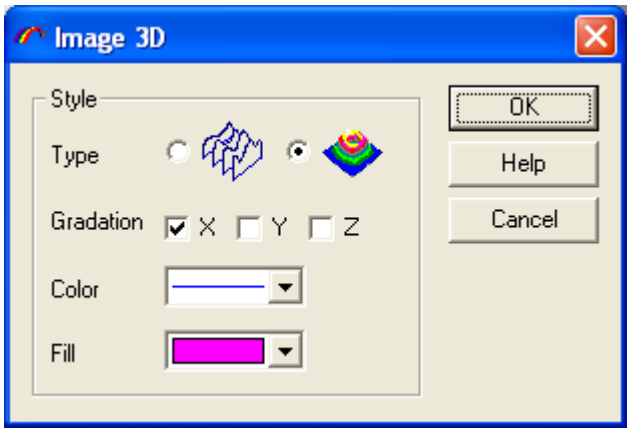


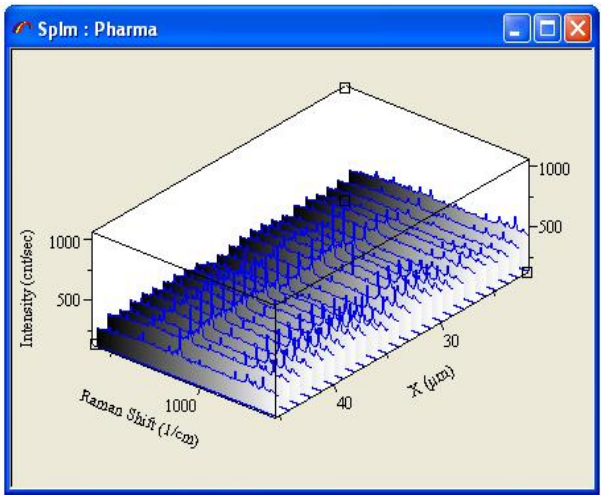
5.3.9- Image3D



The **Image3D Properties** Dialog enables the modification of the appearance of a 3D representation of the data object. To open this dialog, select the Image3D item from the window context menu.

- ✓ **Type** Select between polygon and gradation display mode.
- ✓ **Gradation** Select the axis which defines the direction of the color gradation
- ✓ Click on the **Color** control to modify the polygon border style and color.
- ✓ Click on the **Fill** control to modify the internal polygon fill-style.




SpIm : Pharma
Intensity (cnt/sec)
1000
500
1000
500
Raman Shift (1/cm)
1000
40
30
X (µm)

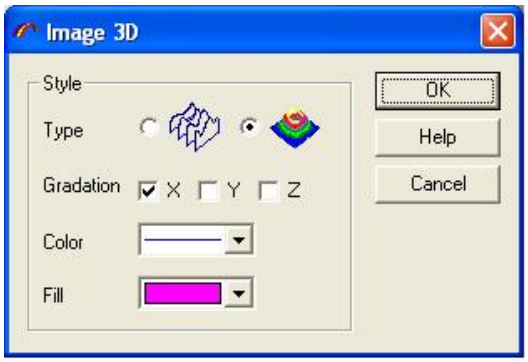


Image 3D
Style
Type
Gradation
X
Y
Z
Color
Fill
OK
Help
Cancel

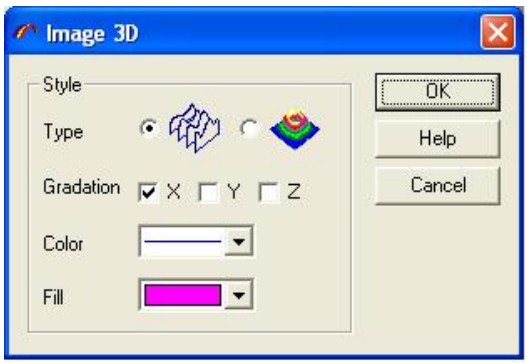
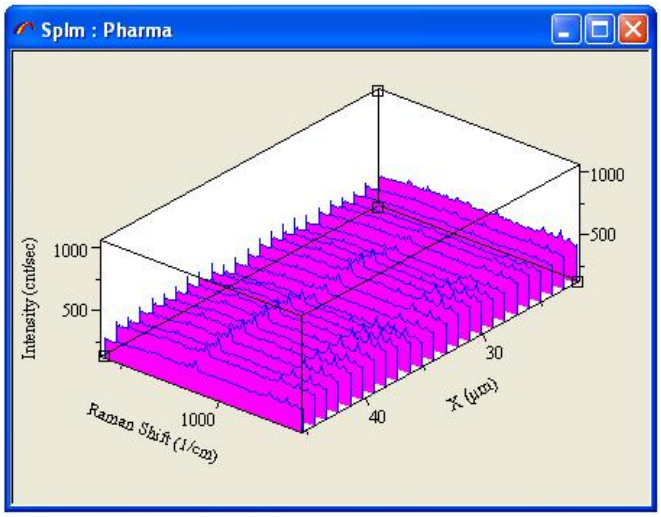


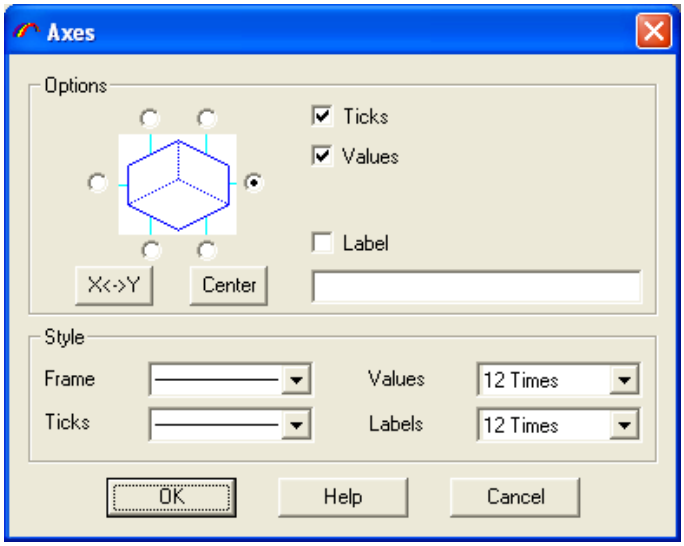
Image 3D
Style
Type
Gradation
X
Y
Z
Color
Fill
OK
Help
Cancel


SpIm : Pharma
Intensity (cnt/sec)
1000
500
1000
500
Raman Shift (1/cm)
1000
40
30
X (µm)

5.3.10- 3Daxes

The **3D Axes Dialog** allows you to modify the appearance of the axes for 3D representation of data objects. You access to this Axes dialog by selecting the **Axes** item from the window context menu.

✓ **Options**



First select the axis you wish to customize.

Ticks . Check this box to enable the drawing of ticks.

Values Check this box to enable the display of the number values for ticks.

Label .. Check this box to create the axis output label and edit the label field to customize the axis.

X<>Y .. Click on this button to switch between the X and Y axis.

Center Click on this button to re-center the 3D object in the active window.

✓ **Style**

Frame . Click on the control to modify the color and style of axis edge.
Values. Click on thes control to modify the font values
Ticks ... Click on the control to modify the color and style of the ticks
Labels. Click on the control to modify the labels font

5.4- OTHER FUNCTIONS

5.4.1- Multi (via OPTIONS in the menu bar)

The **Multi** function allows whatever process is performed on the active spectrum to be performed on *all* open spectrum.
For example, if a constant value is added to one spectrum, with **Multi** selected, all the open spectra will have that constant value added to them. This can be a useful way to save a number of files – with **Multi** selected, a save dialog window will appear for each open spectrum, in the order they are displayed in the **Objects** list.

5.4.2- Copy / Paste (Via EDIT in the menu bar)

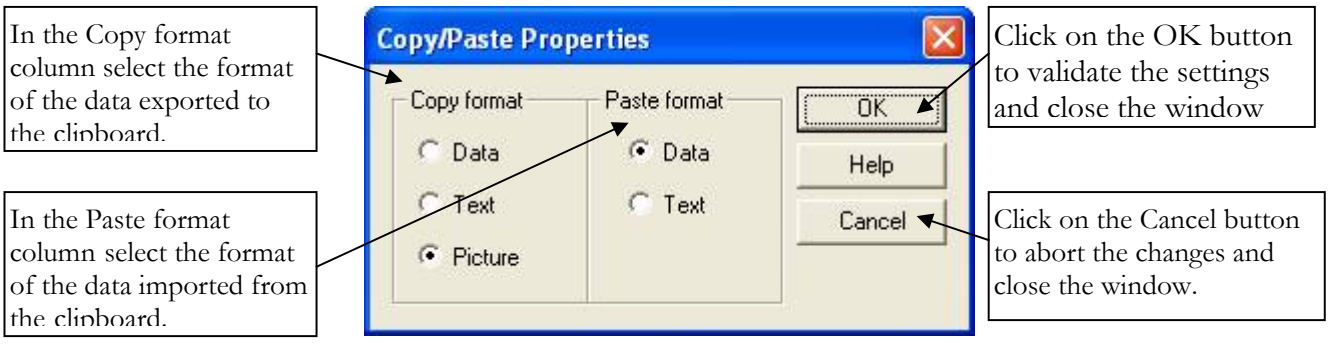
Copy *(CTRL+X)*. To copy the active data in clipboard. You can select the data format with the **Format…** command.

Paste *(CTRL+V)*. To insert the clipboard contents. You can select the clipboard format with the **Format…** command.

Format… To select the **Copy** and **Paste** clipboard data formats.

This command permits to define the format of the data you export to the clipboard or and the one of the data you import from the clipboard.
To access this command select Format… from the Edit commands menu in the Main menu bar.

✓ **The Copy/Paste data formats selection**



- **Data .** Native NextGen format. Can be used to create the exact copy of the data object.
- **Text..** Create the text spreadsheet of the active data object.
- **Picture** Create the screen

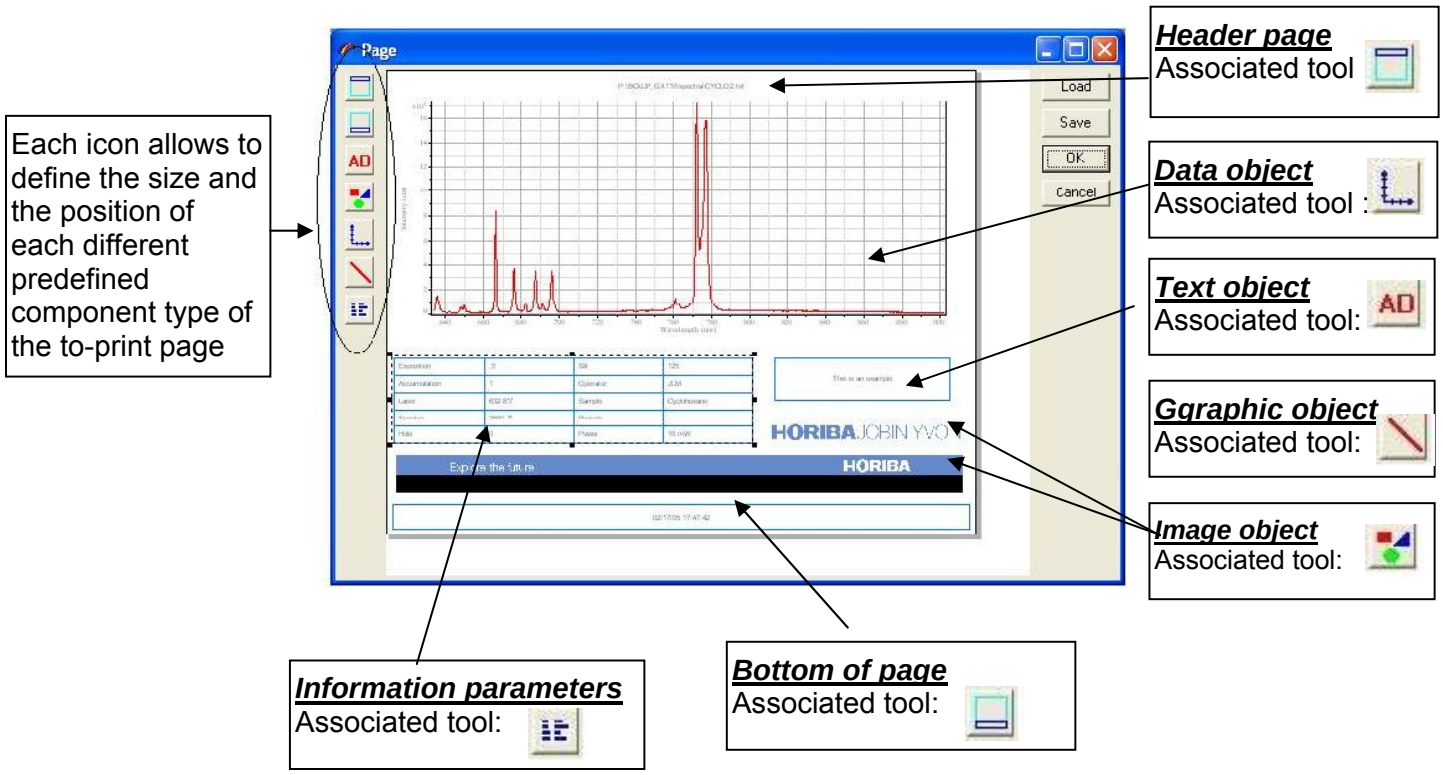
5.4.3- Page Set Up

Page (via FILE in the menu bar) allows the print page to be configured, including the spectrum itself, information from the acquisition, logo, and comments.

✓ **The Page window**

Page tools bar

Components of the to-print page



✓ **The page buttons**

Load To load an already recorded template.

Save To save the current template into a file.

OK To validate the settings and to close the Page window.

Cancel To close the Page window without validating the current Page settings.

✓ **Using the Page tools icons**

To insert a component in the to-print page click on the corresponding tool. Then move the mouse on the page so a cross appears. Then move the cross at the wished location, press on the left mouse button and move the mouse to define the size of the corresponding component.

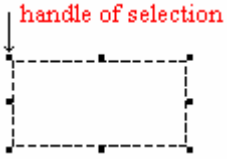
✓ **How to select a component of the to-print page**

Move the mouse on the chosen component and click on the left mouse button. Then a dotted rectangle is displayed around the selected component.

✓ **Moving a component of the to-print page**

Select the component. Then when the following mouse cursor appears, click on left mouse button and drag the mouse.

✓ **Re-sizing a component of the to-print page**

First, click on the object to select it. Selection handles appear around the selected object. 

Move the mouse pointer on one of the selection handles until to have the size pointer: or .Keep the mouse button pressed and move the selection handle and modify the size of the object.

✓ **Modifying or creating the contents of a to-print page component**

Except the data object, the contents of all the other objects could be modified by double-clicking on the wished component.

Then a dedicated window appears with the tools to modify the corresponding component:

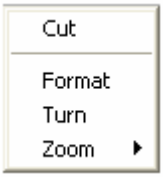
- The ***options*** window for the header page, the bottom of page and the Text object.

-The ***parameters*** window for the array of experiment information parameters.

-The ***Open*** window for the Image object.

✓ **Modifying the general page presentation or display**

Click anywhere on the to-print page on the right button of the mouse to display the following menu



Cut To remove the selected component

Format To define the parameters of the sheet of paper. (See Page Setup)

Turn To define the page orientation Portrait or Landscape

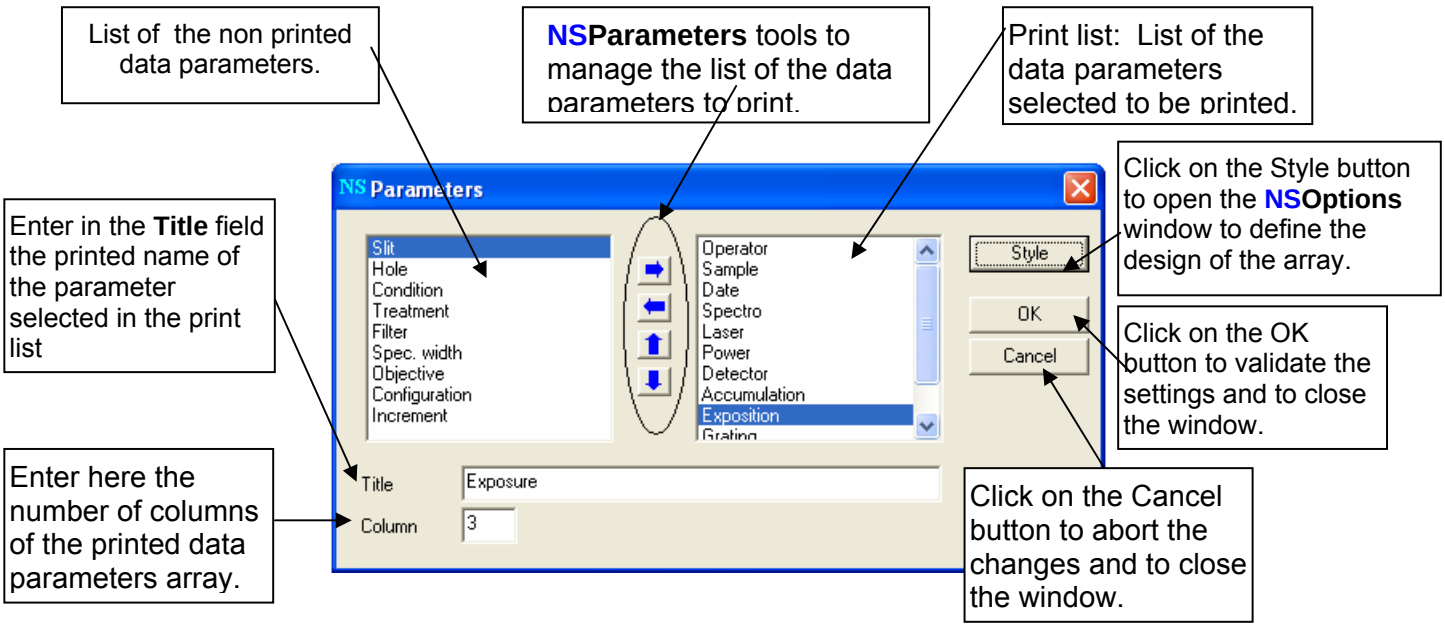
Zoom To define the display of the to-print page inside the ***Page*** window.

✓ **The Parameters function**

On the printed document the selected parameters are laid out in an array. The **Parameters** function permits to select the data parameters you wish to be printed and to define the style of the array.

To access this command double click with the left mouse button on the ***information parameters*** object when defining the layout of the to-print document with the **Page…** command

✓ **The Parameters window**



➢ **Example of a printed data parameters array**

y corresponding to the settings of the **parameters** screen copy as it appears on the printed document.

osure is the printed label for the exposition parameter.

Operator	nf	Laser	784.87	Exposure	40
Sample	acetylsalicylic acid	Power	11.2mw @ sample	Grating	950
Date	6-05-2003 18:55	Detector	CCD4	Remark	
Spectro	312.20	Accumulation	2		

You will find below the data parameters arra

Remark:
A column contains 2 fields: the data parameter label and the data parameter value.

Column 1 | Column 2 | Column 3

➢ **The Parameters tools**

 Add the selected data parameter to the print list.
 Remove the selected data parameter from the print list.
 In the print list move the selected parameter to the previous line.
 In the print list move the selected parameter to the next line.

Icon 1

 : Standard cursor of work

Icon 2

 : Peak elimination

Icon 3

 : Shape correction

Icon 4

 : Zoom

Icon 5

 : Intensity adjustment

Icon 6

 : Shift

Icon 7

 : Manual addition

Icon 8

 : Manual multiplication

Icon 9

 : Manual labeling of peaks

Icon 10

 : Move peak maxima + Fit peak width

Icon 11

 : Delete label of a peak

Icon 12

 : Integral calculation

Icon 13

 : build of a baseline

Icon 14

: delete the point of the baseline

Icon 15

: reduce the size of the graph background ----------

Icon 16

: delete the active object

Icon 17

: open a file

Icon 18

: save a file

Icon 19

: Print page ----------

Icon 20

: Information about object

Icon 21

: object normlalisatiion

Icon 22

: Intensity normalization

Icon 23

: centering of the cursors

Icon 24

: data sizes

Icon 25

 : Informations on the active object

Icon 26

 : Spectrum adjustment

Icon 27

 : CCD image adjustment

Icon 28

 : Spectrum recording

Icon 29

 Spectral images recording

Icon 30

 Automatic Multiwindow spectra recording

Icon 31

Icon 32

 Video image

Icon 33

 : Baseline correction

Icon 34

Correction

Icon 35

 : Filtration

Icon 36 :

 : Fourier filtering

Icon 37

 : Mathematical treatments

Icon 38

 : peak fitting

Icon 39

 : Palette window----------

Icon 40

 : Spectral mapping procedure

Icon 41

 : Profile

Icon 42

 : Model procedure