

# USERS GUIDE



## SR-163



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**SECTION 1 – INTRODUCTION TO THE SHAMROCK SR-163 SERIES**

Firstly thank you for choosing one of Andor's new SR-163 Series spectrographs. We are delighted you have selected our equipment to fulfill your requirements. Here are some of the feature and benefits available to you:

- **Unique design:** the design of the SR-163 spectrograph provides better resolution with higher throughput. It is based on a Czerny-Turner optical layout, features a 163mm focal length and a numerical aperture of  $f/3.6$ .
- **Interchangeable gratings:** gratings can be easily interchanged to suit your wavelength range and resolution requirements with minimal need for re-alignment. A wide selection of various groove frequency gratings is available. The micrometer wavelength drive allows for calibration through the range of wavelengths.
- Interchangeable fixed slits or a variable slit width accessory are also offered to match your resolution/throughput requirements.
- **Robust, compact & accurate:** the SR-163 is built in a solid housing to deliver superior and reliable performance time after time. Its compact size, low cost and versatility make it attractive to researchers and **Original Equipment Manufacturers (OEM's)**.
- **Wide range of accessories available:** the SR-163 is available with a host of input accessories including shutter, input slits or SMA interface, optical fibers & fiber holders and calibration lamps.
- **Flexibility:** the SR-163 base unit can be easily and quickly configured for imaging, multi-track spectroscopy or conventional non-imaging applications. Typical SR-163 typical configurations are shown on the next page. Simply fit the necessary accessories (e.g. shutter, adjustable slit, etc.) to the base unit to convert it easily between modes. Please refer to **pages 15 – 17** for full details of the available accessories.
- Available for use with a wide range of cameras: including CCD's, EMCCD's and ICCD's. Also available as a stand-alone option for use with existing or third party detectors.
- **Carefully designed baffling:** coupled with tilted detector flange minimizes back reflection and stray light from the detector window.
- **Convenient mounting configurations:** enable the unit to be set-up according to the working environment.

**NOTE: Before removing the SR-163 from its packaging, please refer to page 16.**

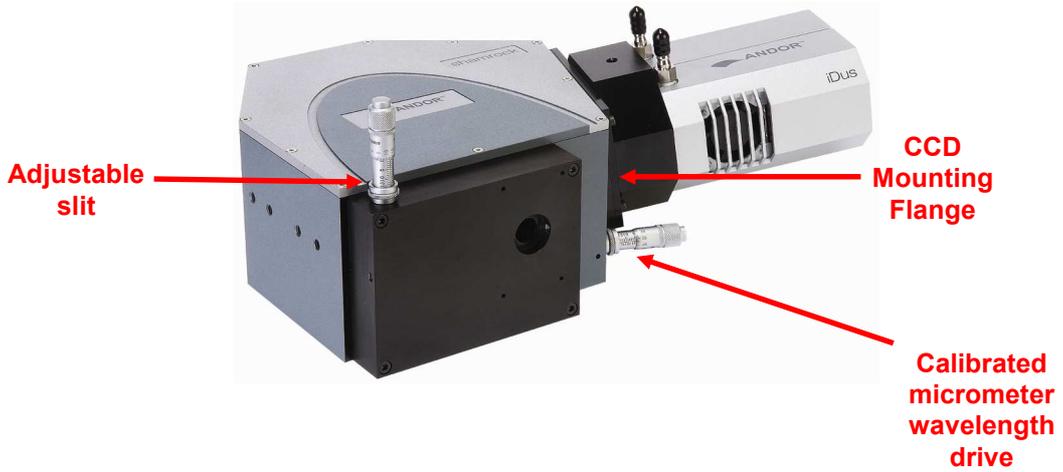


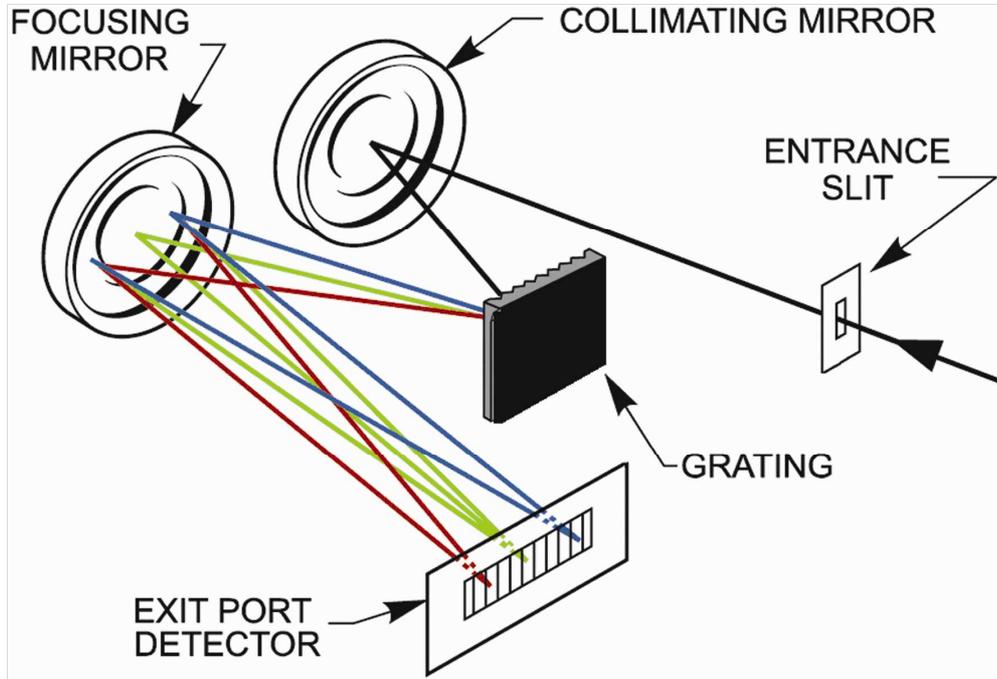
Figure 1: SR-163 configured as a non-imaging spectrograph



Figure 2: SR-163 configured as an imaging spectrograph

1.1 - SR-163 SERIES PRINCIPLES

The SR-163 is based around a Czerny-Turner spectrograph configuration. This makes use of mirrors as focusing & collimating devices in an off-axis configuration. It employs a planar reflective grating in the collimated space, as illustrated below:



The single spectrograph design and is very compact and inexpensive.

1.1.1 - Wavelength Drive

The wavelength drive is a direct sine drive. This ensures the highest degree of wavelength repeatability and minimizes any backlash. The micrometer is calibrated to read 1nm per 10µm of travel for a 1200 g/mm grating (it will read half the true wavelength with a 600 g/mm grating).

**Example**

The calibrated wavelength is that at the center of the array, thus when the micrometer reads 703nm, the true wavelength is 703nm (with a 1200 l/mm grating).

**NOTE:** Unless otherwise stated, the specifications are obtained with a 1200l/mm grating.

<b>General</b>	Czerny-Turner arrangement
<b>Focal length (mm)</b>	163
<b>Aperture ratio (F#)</b>	F/3.6
<b>Focal plane size (mm W x H)</b>	28 x 10
<b>Mechanical scan range (nm)</b>	0 - 1275
<b>Reciprocal dispersion (nm/mm) nominal</b>	4.43
<b>Wavelength accuracy (nm)</b>	± 0.25
<b>Wavelength resolution (nm)<sup>1</sup></b>	0.17
<b>Vertical magnification</b>	1.8
<b>Horizontal magnification</b>	1
<b>Optical axis height (mm)</b>	55.9
<b>Stray light</b>	$2 \times 10^{-4}$ (measured at 20nm from 633nm laser line)
<b>Size in mm (typical SR-163 configuration)</b>	197.2 x 218.1 x 95.9
<b>Size in mm ( typical SR-163i configuration )</b>	210 x 218.1 x 95.9
<b>Weight in kg ( typical SR-163 configuration )</b>	3.5
<b>Weight in kg ( typical SR-163i configuration )</b>	3.9
<b>Grating size (mm)</b>	40 x 40

<sup>1</sup> Measured with 10µm slit and 13.5µm pixel size CCD

**1.3 - WORKING WITH THE USERS GUIDE**

This manual is aimed at experienced researchers who will be using their SR-163 to analyse samples spectroscopically and also for imaging applications.

We hope you find using our product easy & beneficial. However, if you have any suggestions as to how our software, hardware or documentation could be improved, we would be pleased to hear from you. Contact details of your nearest representative can be obtained on **page 12**.

**1.4 - DISCLAIMER**

**The information contained herein is provided "as is" without warranty, condition or representation of any kind, either express, implied, statutory or otherwise, including but not limited to, any warranty of merchantability, non-infringement or fitness for a particular purpose.**

**In no event shall Andor be liable for any loss or damage, whether direct, indirect, special, incidental, consequential or otherwise howsoever caused whether arising in contract tort or otherwise, arising out of or in connection with the use of the information provided herein.**

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2. The publication of information in this documentation does not imply freedom from any patent or proprietary right of **Andor Technology plc** or any third party.

**1.5 - TRADEMARKS & PATENT INFORMATION**

Andor, the Andor logo and **Shamrock SR-163** are all trademarks of **Andor Technology plc**.

All other marks are property of their owners.

Changes are periodically made to the product and these will be incorporated into new additions of the manual.

**1.6 - TECHNICAL SUPPORT**

If you have any questions regarding the use of this equipment, please contact the representative from whom your system was purchased, or:

<p><b>Europe</b></p> <p><b>Andor Technology</b>            7 Millennium Way            Springvale Business Park            Belfast            BT12 7AL            Northern Ireland            Tel. +44 (0)28 9023 7126            Fax. +44 (0)28 9031 0792  <b>e-mail: productsupport@andor.com</b></p>	<p><b>USA</b></p> <p><b>Andor Technology</b>            425 Sullivan Avenue - Suite 3            South Windsor            CT 06074            USA            Tel. +1 (860) 290-9211            Fax. +1 (860) 290-9566  <b>e-mail: productsupport@andor.com</b></p>
<p><b>Asia-Pacific</b></p> <p><b>Andor Technology (Japan)</b>            7F Ichibancho Central Building            22-1 Ichiban-Cho            Chiyoda-Ku            Tokyo 102-0082            Japan            Tel. +81-3-3511 0659            Fax. +81-3-3511 0662  <b>e-mail: productsupport@andor.com</b></p>	<p><b>China</b></p> <p><b>Andor Technology</b>            Room 1116            Zhejiang Building            No. 26            An Zhen Xi Li            Section 3            Chaoyang District            Beijing 100029            China            Tel. +86-10-5129-4977            Fax. +86-10-6445-5401  <b>e-mail: productsupport@andor.com</b></p>

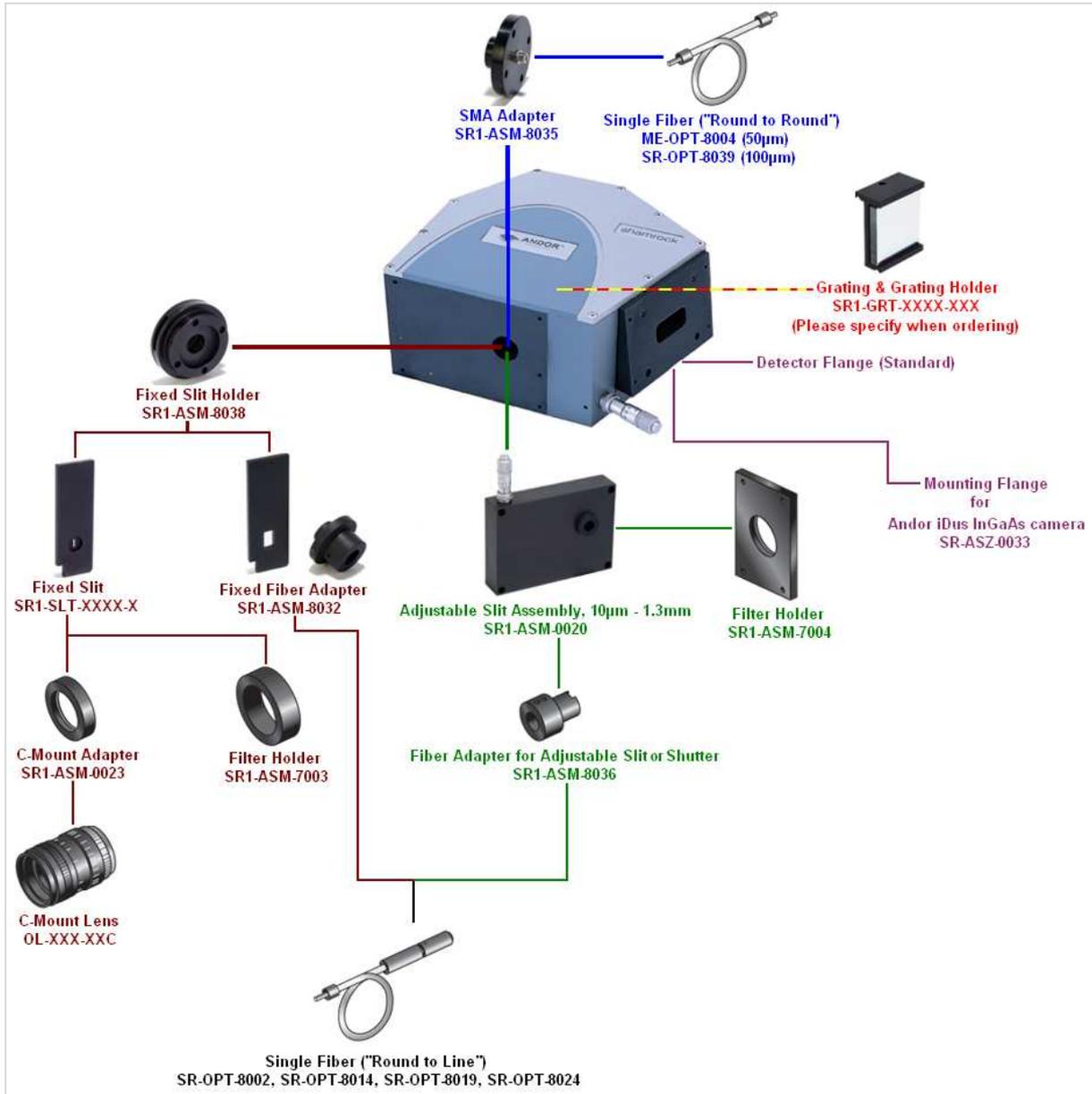
**\*NOTE: THE CONTACT DETAILS FOR YOUR NEAREST REPRESENTATIVE CAN BE FOUND ON OUR WEBSITE.**

**SECTION 2 - ACCESSORIES**

A wide range of accessories is available as shown below and on the next page.

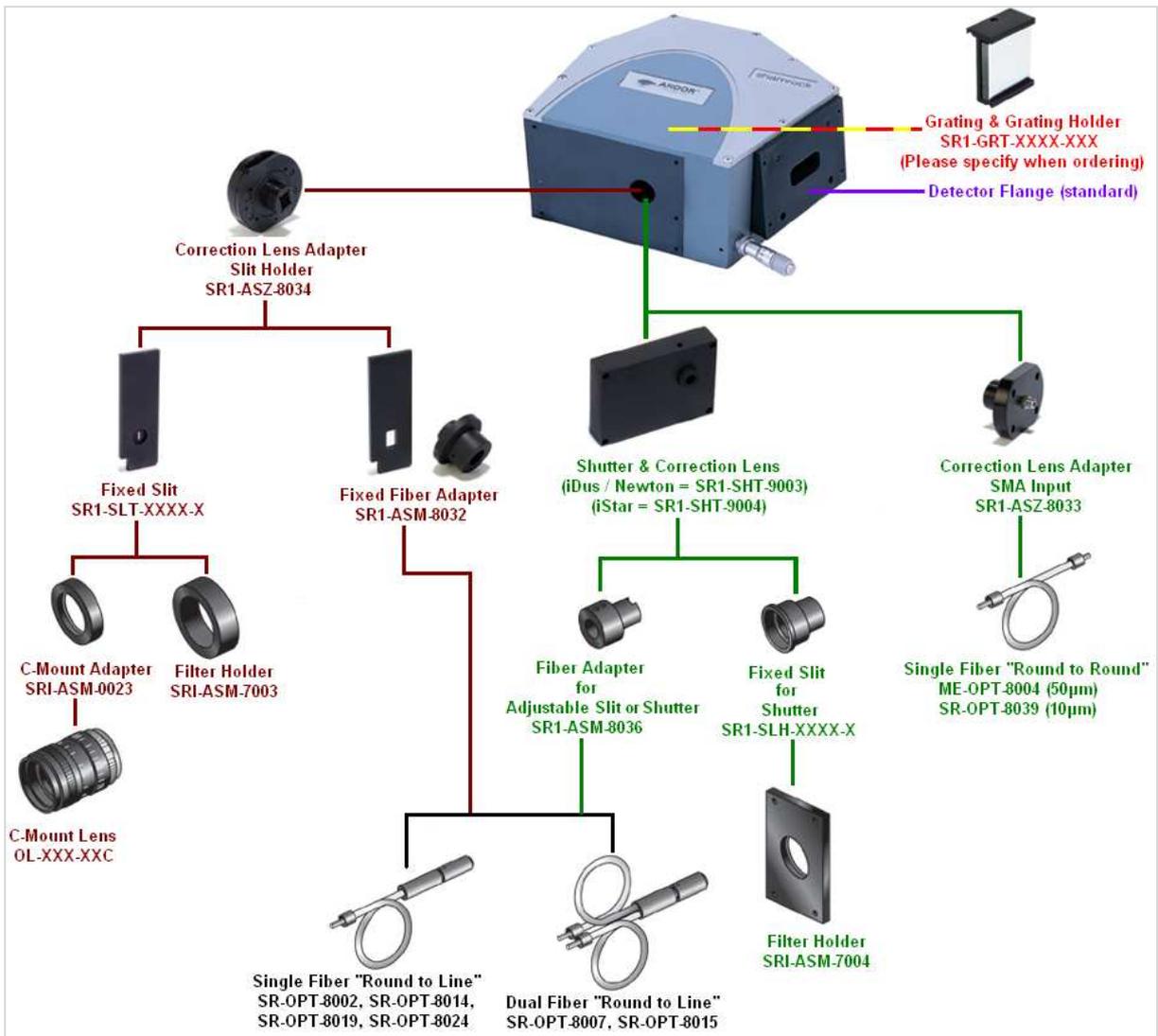
**2.1 - SPECTRAL MODE ACCESSORIES**

The accessories available to configure the SR-163 for spectroscopy applications is shown here:



**2.2 - IMAGING MODE ACCESSORIES**

The accessories available to configure the SR-163 for imaging applications is shown here:



**2.3 - ACCESSORIES TABLE FOR THE SR-163 SERIES**

Part No.	Description	Remarks
SR1-GRT-XXXX-XXX	Grating & Grating Holder	Must be specified when ordering
SR-ASM-0014	Pen Ray Holder	
<b>FIXED SLIT INPUTS &amp; ADAPTERS</b>		
OL-XXX-XXC	C-Mount Lens	Various sizes available - please call for details
SR1-ASM-0023	C-Mount Adapter	
SR1-ASM-7003	Filter Holder	
SR1-ASM-8032	Fixed Fiber Adapter	For Andor Ferrule Fibers
SR1-ASM-8038	Fixed Slit Holder	
SR1-ASZ-8034	Correction Lens Adapter Slit Input	
SR1-SLT-XXXX-X	Fixed Slit	Various sizes available - please call for details
<b>ADJUSTABLE SLITS &amp; ADAPTERS</b>		
Part No.	Description	Remarks
SR1-ASM-0020	Adjustable Slit Assembly (10µm – 1.3mm)	
SR1-ASM-8036	Fiber Adapter for Adjustable Slit & shutter	
SR1-ASM-7004	Filter Holder	
<b>SMA MOUNTS &amp; ADAPTERS</b>		
Part No.	Description	Remarks
SR1-ASZ-8033	Correction Lens Adapter SMA Input	
SR1-ASM-8035	SMA Adapter	
<b>SHUTTERS &amp; ADAPTERS</b>		
Part No.	Description	Remarks
SR1-SHT-9003	Shutter & Corrections Lens for iDus & Newton cameras	
SR1-ASM-8036	Fiber Adapter for Adjustable Slit & Shutter	
SR1-SLH-XXXX-X	Fixed Slit for Shutter	Various sizes available - please call for details
SR1-ASM-7004	Filter Holder	
<b>FIBERS*</b>		
ME-OPT-8004	1 way "Round –To-Round" 50µm core (UV)	SMA - SMA
SR-OPT-8002	1 way "Round-To-Line" type 100µm core (LOH-VIS/NIR)	Common to Slit & Shutter mounts
SR-OPT-8007	2 way "Round-to-Line" 100µm core (LOH-VIS/NIR)	Common to Slit & Shutter mounts
SR-OPT-8014	1 way "Round-To-Line" 100µm core (HOH-UV/VIS)	Common to Slit & Shutter mounts
SR-OPT-8015	2 way "Round-to-Line" 100µm core (HOH-UV/VIS)	Common to Slit & Shutter mounts
SR-OPT-8019	2 way "Round-To-Line" 200µm core (LOH-VIS/NIR)	Common to Slit & Shutter mounts
SR-OPT-8024	1 way "Round-To-Line" 200µm core (HOH-UV/VIS)	Common to Slit & Shutter mounts
SR-OPT-8039	1 way "Round –To-Round" 100µm core (LOH-VIS/NIR)	

\* Other fibers are available on request

**SECTION 3 - INSTALLATION****3.1- UNPACKING THE SR-163**

Before unpacking the instrument, allow the shipping box to fully acclimatize to room temperature.

Whilst the SR-163 requires no special placement in a controlled environment, it should be noted that it is a precision instrument that will perform best when set up and operated properly. Please read this manual carefully before using and always handle with the care accorded to any precision instrument.

Carefully remove the SR-163 from its packaging. The following should be included:

- SR-163 base unit and relevant accessories
- Allen key (wrench) set comprising 2mm, 2.5mm & 3mm keys
- Users guide (this publication) and Performance Sheet

Depending on the options purchased the following may also be included:

- Andor camera (for connection to the SR-163)

The following pages show how to mount the spectrograph and also fit many of the accessories shown previously in **Section 2**.

**3.2 - SAFETY PRECAUTIONS**

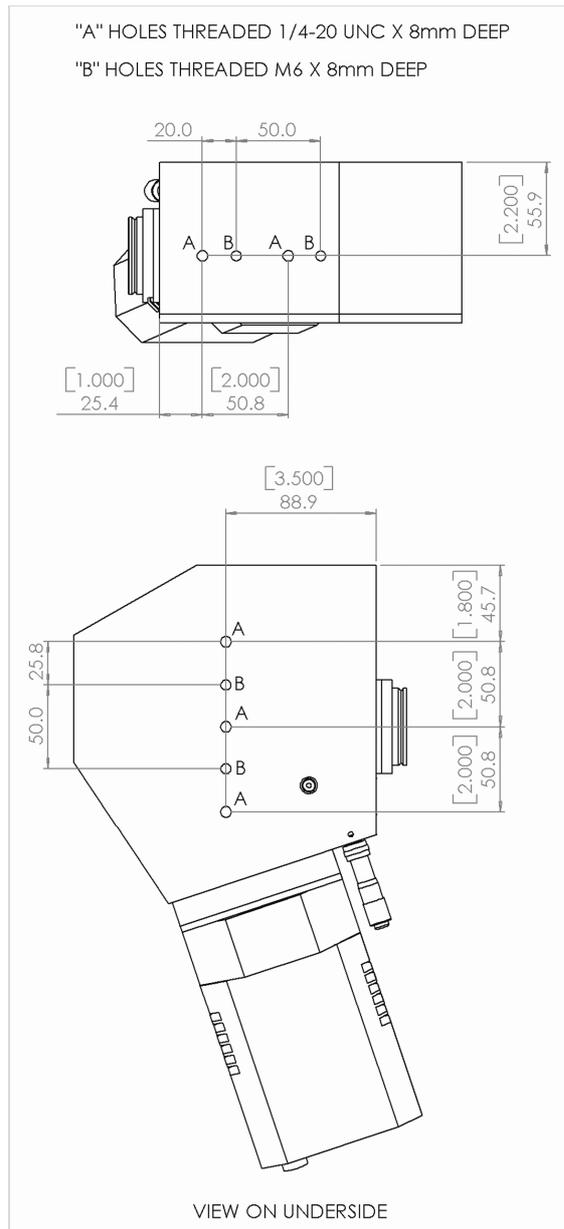
**There are no user-serviceable parts inside the SR-163. Care should be taken when working around the front surface optics.**

**NOTE: THE COVER SHOULD ONLY BE OPENED WHEN ABSOLUTELY NECESSARY, I.E. TO SWAP OUT GRATING TURRETS OR OTHER ACCESSORIES. PLEASE SEE PAGES 20 - 22 FOR DETAILS OF HOW TO REMOVE THE LID, SAFELY CHANGE GRATINGS OR ADJUST THE COLLIMATING MIRROR HEIGHT.**

## 3.2.1 - Base Unit Mounting

The SR-163 is easily mounted to a variety of surfaces. There are four ways to mount it as follows:

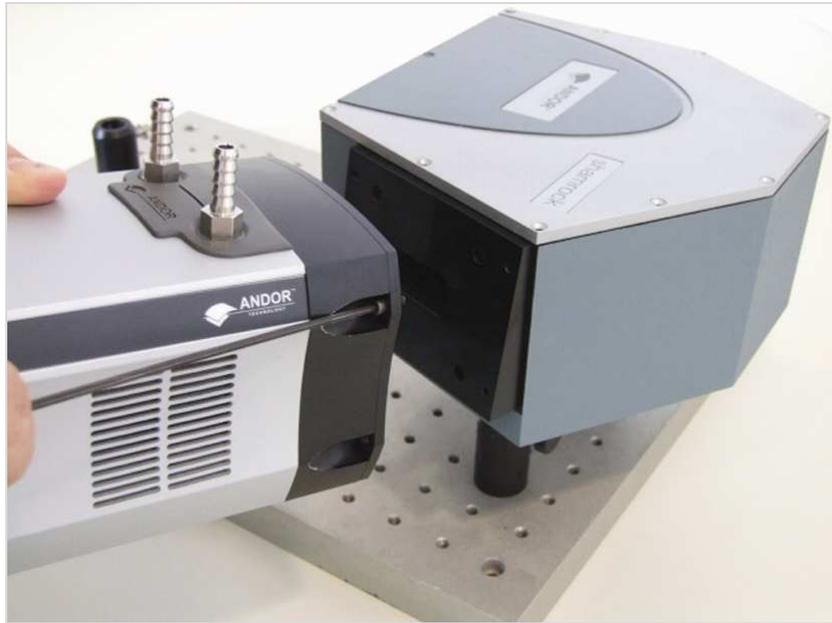
- 5-off 1/4 -20 UNC x 8mm holes are located 2x on the side of casing for vertical integration and 3x underneath for horizontal operation. These are marked **A** on the diagram below.
- 4-off M6 x 8mm tapped holes are located 2x under the casing for horizontal operation and 2x on the side for vertical integration. These are marked **B** on the diagram below.



- The SR-163 can be conveniently mounted using the 1.5" (46mm) diameter male flange of the entrance slit holder.
- Coupling blocks are available on special request for mounting the spectrograph onto different surfaces. Please contact us for further details.

**3.2.2 - Connecting a camera to the SR-163**

The Andor camera is connected to the SR-163 using the attached flange supplied with the product, e.g.:



**NOTE: 4-off 3/32 x 1/8 UNC screws are required to secure the camera. An Allen wrench is supplied for this purpose.**

The rest of this section describes how to change gratings, adjust the mirror and install various accessories.

A wide range of replicated plane reflection and holographic gratings are available. Gratings can be chosen to optimize efficiency over a wavelength region or to have different dispersion resolution properties. The grating is field-replaceable; the pre-aligned mount simply drops into place. **NOTE: Before you install a new grating, please ensure you have selected the correct type from the table below.**

l/mm	Blaze (nm)	Dispersion (nm/mm) <sup>4</sup>	Bandpass <sup>1</sup>	Resolution <sup>2</sup> (nm) @ 546nm	Andor Part No.
150	300	40.21	1110	1.57	SR1-GRT-0150-0300
150	500	40	1104	1.36	SR1-GRT-0150-0500
200	730	29.87	824	1.16	SR1-GRT-0200-0730
300	300	20.1	555	0.78	SR1-GRT-0300-0300
300	500	19.9	549	0.77	SR1-GRT-0300-0500
300	760	19.61	541	0.76	SR1-GRT-0300-0760
300	860	19.48	538	0.76	SR1-GRT-0300-0860
400	400	14.9	411	0.58	SR1-GRT-0400-0400
400	550	14.73	407	0.57	SR1-GRT-0400-0550
400	850	14.34	396	0.56	SR1-GRT-0400-0850
500	330	11.91	329	0.46	SR1-GRT-0500-0330
500	560	11.63	321	0.45	SR1-GRT-0500-0560
500	770	11.34	313	0.44	SR1-GRT-0500-0770
600	300	9.896	273	0.38	SR1-GRT-0600-0300
600	500	9.65	266	0.38	SR1-GRT-0600-0500
600	750	9.29	256	0.37	SR1-GRT-0600-0750
900	550	6.11	169	0.24	SR1-GRT-0900-0550
1200	300	4.76	132	0.18	SR1-GRT-1200-0300
1200	500	4.43	122	0.17	SR1-GRT-1200-0500
1200	750	3.89	107	0.16	SR1-GRT-1200-0750
1800 <sup>3</sup>	500	2.59	71	0.1	SR1-GRT-1800-0500
2400 <sup>3</sup>	300	2.12	59	0.08	SR1-GRT-2400-0300

<sup>1</sup> Measured for a 27.6mm wide CCD

<sup>2</sup> Resolution measured with 10µm slit and 13.5 µm pixel size CCD

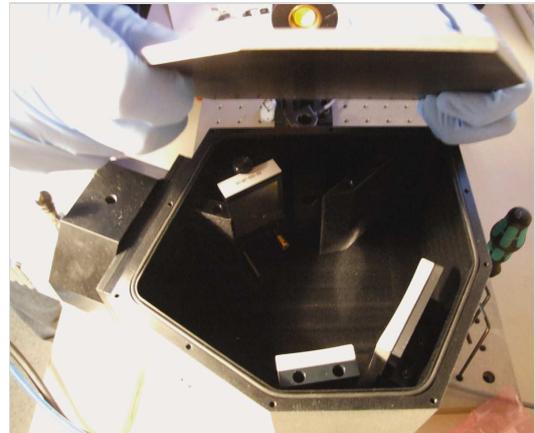
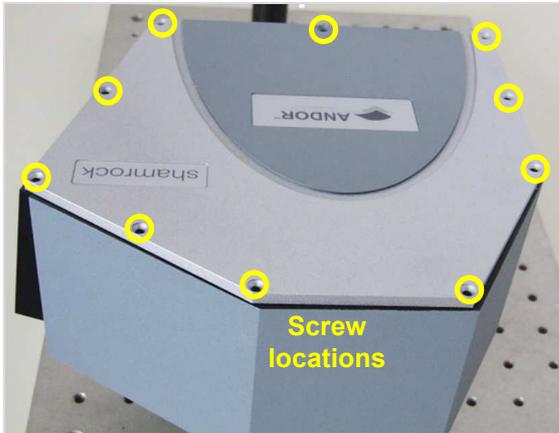
<sup>3</sup> The upper wavelengths of 1800 l/mm and 2400 l/mm gratings are limited by the spectrograph mechanics to 750nm & 540nm respectively

<sup>4</sup> Dispersion calculated @ blaze wavelength

**NOTE: Other special groove frequency and blaze wavelength gratings are available on request.**

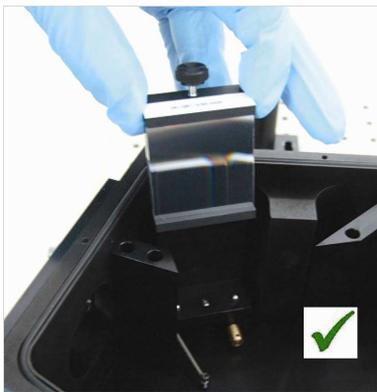
**NOTE:** We recommend you wear protective gloves at all time during this procedure.

**Step 1:** Unscrew the 10-off hexagonal head CSK screws with 2.5mm Allen key and remove lid:



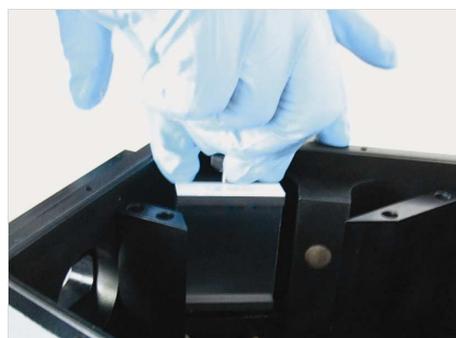
**Step 2:** Remove grating (handling as shown below left) and carefully place it in an appropriate protective cover:

**NOTE: DO NOT HANDLE THE GRATING AS SHOWN HERE:**



**IF THE GRATING IS HELD BY THE FIXING SCREW, IT CAN COME DETACHED. THE ASSEMBLY GRATING COULD THEN DROP AND BE DAMAGED.**

**Step 3:** Place the new grating onto the 4-off ball-bearing mounts (shown ringed below), making sure it is correctly inserted into the locating groove, then tighten the screw:



**Step 4:** Replace lid, making sure the O-ring is correctly in place then tighten the 10-off hexagonal screws.

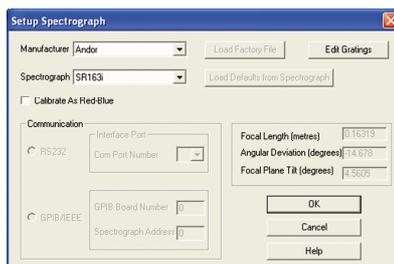
## 3.2.4 - Coarse Center Wavelength Micrometer Setting

Before you can perform a calibration using the SR-163, you must ensure that the system is setup in software.

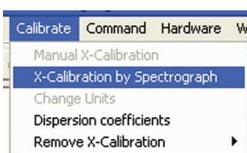
1. Select the **Setup Spectrograph** option from the **Hardware** menu:



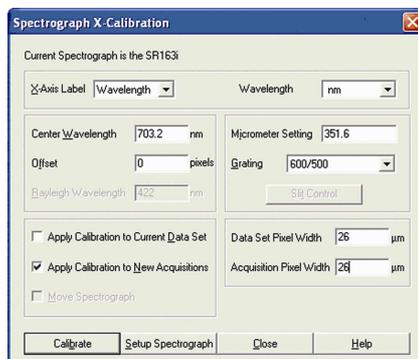
The **Setup Spectrograph** dialog box will appear, e.g.:



2. Select **Andor** from the **Manufacturer** drop-down menu and **SR163** from the **Spectrograph** drop-down menu then click **OK**.
3. Select the **X-Calibration by Spectrograph** option from the **Calibrate** menu:



The **Spectrograph X-Calibration** dialog box will appear e.g.:



4. Set the micrometer to the figure\* which is then shown in the **Micrometer Setting** field.

\* **NOTE: Please refer to the table on page 19, as this figure may not be obtainable. The standard micrometer calibration is for 1200l/mm Grating.**

## 3.2.5 - Adjusting Mirror

The mirror inside the unit can be adjusted to suit the height of the signal on the CCD as it may vary for grating to grating. **NOTE: Check the height of the grating on the CCD before carrying out this adjustment.**

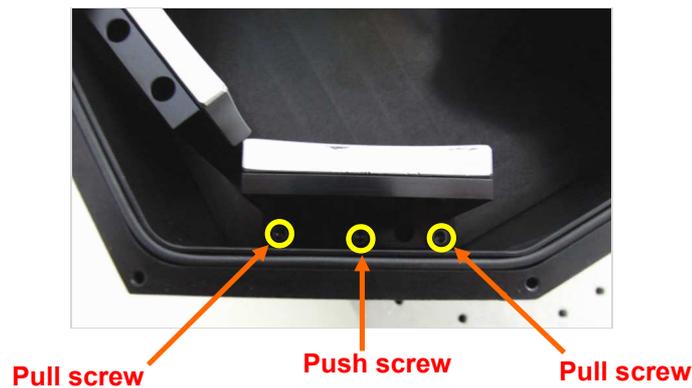
The procedure is as follows

**Step 1:** Remove the lid as shown on **page 20**.

**Step 2:** Adjust the Cap head push/pull mirror adjustment screws as shown here:



Ensure all 3 screws are securely in contact with the mount at the end of the adjustments. This ensures better stability over time. The location of the mirror adjustment screws is shown below:



**Step 3:** Replace lid.

## 3.2.6 - SR1-ASZ-8034 / SR1-ASZ-8038 (Correction Lens Adapter Slit Input / SMA Input)

**Step 1:** Remove protective film, cover & O-ring holders from Slit Holder / SMA Input:



**NOTE:** Use a dry air line to remove any dust from the lens if necessary.

**Step 2:** Make sure the O-ring is still correctly fitted. Place the Slit input or SMA Input into the spectrograph slot with thin end towards spectrograph and tighten the 4-off M2.5 x 20 countersunk screws with a 2mm Allen key, e.g.:



**NOTE:** Before you install a fixed slit, please ensure you have selected the correct type as shown in this table:

Slit width ( $\mu\text{m}$ )	Slit height (mm)	Resolution (nm) @ 546nm**	Andor Part Number
10	3	0.17	SR1-SLT-0010-3
25	3	0.28	SR1-SLT-0025-3
50	3	0.46	SR1-SLT-0050-3
75	3	0.58	SR1-SLT-0075-3
100	3	0.69	SR1-SLT-0100-3
200	3	1.1	SR1-SLT-0200-3
50	3	2.0	SR1-SLT-0500-3

\*\* Resolution measured with 1200 l/mm grating and 13.5  $\mu\text{m}$  pixel size CCD

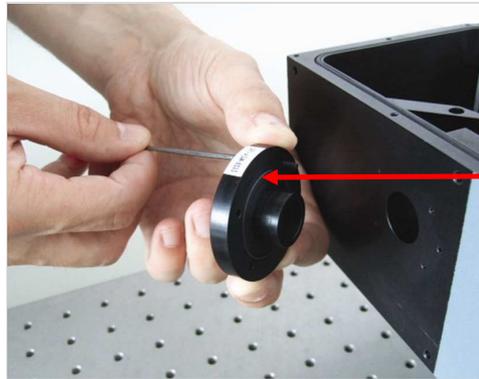
Figure 5 shows placing a Fixed Slit into the top of the Slit Input:



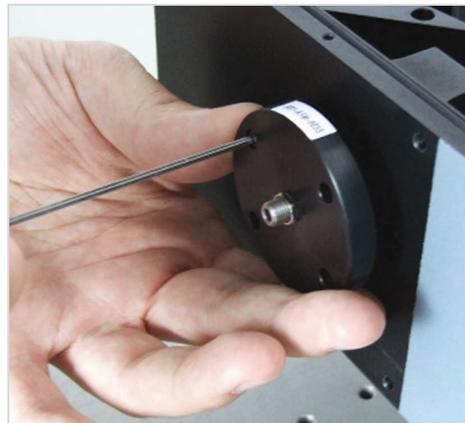
## 3.2.7 - SR1-ASM-8035 / SR1-ASM-8038 (SMA Adapter / Fixed Slit Holder)

**Step 1:** Remove the protective cap from the adapter.

**Step 2:** Place the adapter (SR1-ASM-8035 shown in this example) in the spectrograph slot and tighten the 4-off M2.5 x 8 Cap head screws:



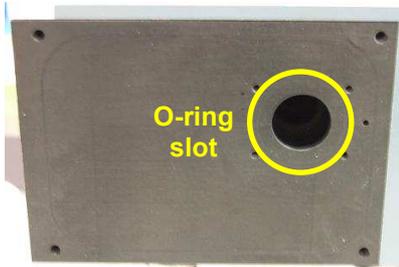
Ensure O-ring  
Is still in place



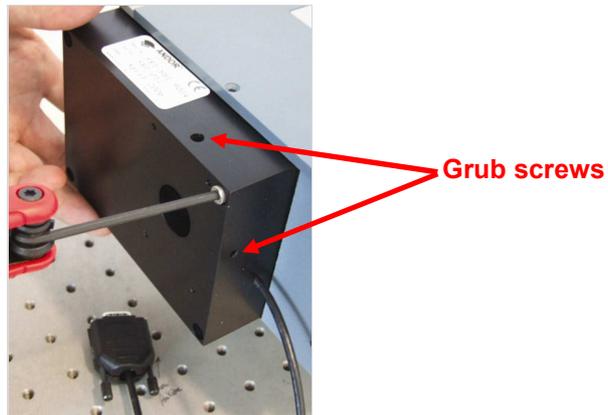
## 3.2.8 - SR1-SHT-9003 & SR1-SHT-9004 (Shutter and Correction Lens Assemblies)

**Step 1:** Remove any other accessories that are installed on the SR-163.

**Step 2:** Ensure the large O-ring is removed, then place the shutter assembly in spectrograph as shown:



**Step 3:** Screw in using 4-off M4 x 30 Cap head screws, then adjust the fiber as required using the grub screws on the top and right side of the shutter assembly



**Step 4 :** Depending on the type of shutter, connect the cable either to the PCI card on the PC or directly to the I2C socket on the rear of camera as shown below:



Figure 1: Connecting I<sup>2</sup>C shutter control cable from SR1-SHT-9003 shutter directly to camera



Figure 2: Connecting shutter control cable from SR1-SHT-9004 shutter to PCI card

**3.2.9 - SR1-ASM-8032 (Fixed Fiber Adapter)**

**Step 1:** Install the **SR1-ASM-8032** holder as per the instructions for fitting the **SR1-ASZ-8034/8038** (shown on page 23) and insert the **Clearance Separator** (part # **SR1-ASM-8032-A**):



**Step 2:** Place the Adapter (part # **SR1-ASM-8032-B**) in the Slit Holder:



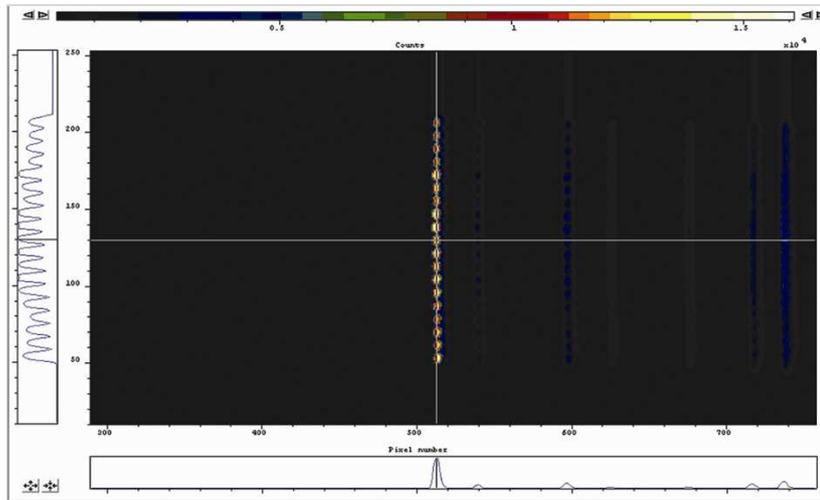
**Step 3:** Push the Adapter as far as it will go. Orientate the adapter as necessary, then tighten the grub screw



**Step 4:** Insert the fiber:



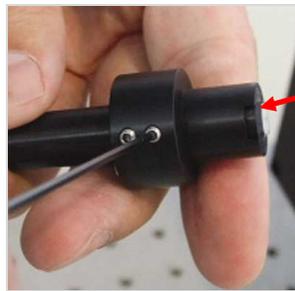
**Step 5:** With the **SOLIS** software in **Imaging** mode, rotate the detector until the image is lined up with the cross-hairs, e.g.:



**Step 1:** Place the fiber into the Fiber Adapter:



**Step 2:** Tighten the 4-off M3 nylon tipped grub screws:



**Ensure fiber is pushed in fully (N.B. it protrudes by 1mm)**

**Step 3:** Insert the Adapter into the front of shutter assembly. Adjust rotation and focus then lock the nylon tipped grub screw on the side:





**Step 1:** Remove any other accessories fitted to the SR-163

**Step 2:** Loosely attach assembly using 4-off M4 x 25 cap head screws.

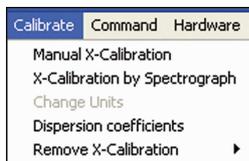
**Step 3:** Couple light source to spectrograph

**Step 4:** Image signal in real-time with detector and adjust housing orientation with a spectral line, then secure the screws.

## SECTION 4 - CALIBRATION

## 4.1 - INTRODUCTION TO CALIBRATION

The following calibration options for data displays are available from the **Calibration** Menu on the Main Window:



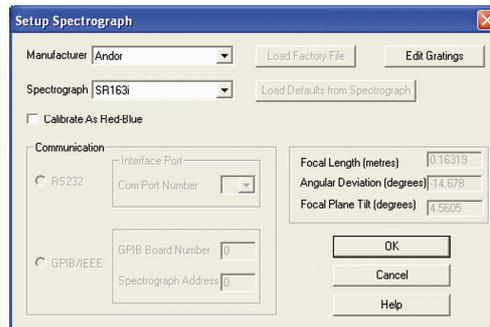
- **X-Calibration by Spectrograph:** lets you calibrate the x-axis of your data displays with reference to your spectrograph's specifications. Calibration may be in wavelength or Raman shift.
- **Manual X-Calibration:** lets you calibrate the x-axis of data displays by manually setting values (time, pixel number, wavelength, Raman shift or spatial position) against recognizable features of a particular 2D data trace.
- **Change Units:** lets you change the units on the x-axis of a data display (e.g. **nm** to **µm**, **cm** to **pixel number**, etc.)
- **Dispersion coefficients:** these are calculated for individual systems and the figures can be found on a label on the side of the SR-163.
- **Remove X-Calibration** (has the following two options):
  1. **Current Data:** returns the data in the active Data Window to its default pixel x-calibration.
  2. **New Acquisitions:** causes future data to be acquired with the default pixel x-calibration.

**4.1.1 - Setup Spectrograph**

Before you can perform a calibration using the SR-163, you must ensure that the system knows which spectrograph you are using. Select the **Setup Spectrograph** option from the **Hardware** menu:



The Setup Spectrograph dialog box will appear, e.g.:



Select **Andor** from the **Manufacturer** drop-down menu and **SR163** from the **Spectrograph** drop-down menu then click **OK**.

**NOTE:** The figures in the Focal Length (metres), Angular Deviation (degrees) and Focal Plane Tilt (degrees) boxes are set as per the performance sheet. Future version of Solis software will allow the user to change these figures.

**4.1.1.1 - Calibrate as Red-Blue**

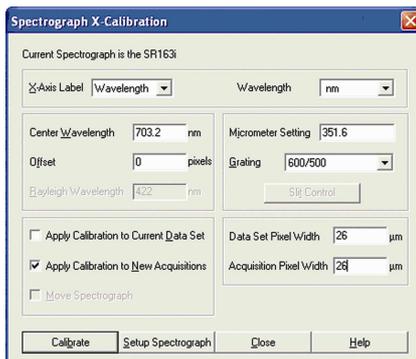
Some CCD detectors readout data in the reverse direction to Andor cameras. In this case, the longer wavelengths (red) are to the left (as viewed from the detector), and shorter wavelengths (blue) are to the right. If you tick the **Calibrate As Red-Blue** option in the **Setup Spectrograph** dialog box, the system then uses software to “reverse” the output of the detector when it generates a data window, thus presenting the display in the more usual orientation.

4.2 - X-CALIBRATION BY SPECTROGRAPH

To calibrate data using the spectrograph select the **X-Calibration by Spectrograph** option from the **Calibrate** menu:



The **Spectrograph X-Calibration** dialog box will appear e.g.:



Ensure that the current spectrograph is set as SR163. If it is not, click on the **Setup Spectrograph** button at the bottom of the page and the **Setup Spectrograph** dialog box will appear. Set the spectrograph as shown on the previous page.

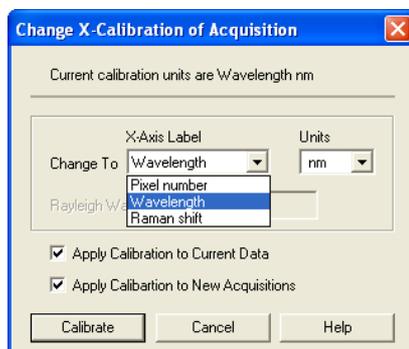
4.2.1 - X-Axis Label & Units

The Spectrograph X-Calibration Dialog box allows you to select, from scrollable drop-down list boxes, an **X-Axis Label** for your data window and an appropriate **Unit** of measurement.

The following label & unit combinations are available:

X-Axis Label	Units
Wavelength	nm, $\mu\text{m}$ , $\text{cm}^{-1}$ , eV
Raman Shift	$\text{cm}^{-1}$

To change the x-axis units of an active data window which you have previously calibrated, select the Change Units option on the Calibrate Menu. The **Change X-Calibration of Acquisition** dialog box will appear e.g.:



From the **X-Axis Label** drop-down list choose whether you want the x-axis to represent **Wavelength**, **Pixel Number** or **Raman Shift**.

From the **Units** drop-down list, choose the units that you want to use for your recalibration.

The available combinations depend on how the data were previously calibrated. If for instance, the data were previously calibrated in Wavelength and Nanometers the available combinations for recalibration are:

<b>Wavelength</b>	nm, $\mu\text{m}$ , $\text{cm}^{-1}$ , eV
<b>Raman Shift</b>	$\text{cm}^{-1}$
<b>Pixel Number</b>	-

**Table 1** shows the available combinations for all modes.

Table 1: Label & Unit changes

	X-Axis Label	Units	Can Change to
0	User Type	-	
1	*Pixel Number (see <b>NOTE 1</b> below)	-	
2	Wavelength	nm, $\mu\text{m}$ , $\text{cm}^{-1}$ , eV	1, 2, 3
3	Raman Shift	$\text{cm}^{-1}$	1, 2
4	Position	$\mu\text{m}$ , mm, cm, $\mu\text{i(nches)}$ , in(ches)	1, 4
5	Time	ms, s	1, 5
6	Sample	-	1

### NOTES:

1. Changing from pixel number actually constitutes a new calibration and can only be performed by using **Manual X-Calibration** or **X-Calibration by Spectrograph**.
2. If you choose to recalibrate a data window in pixels, you will not be able to perform any further recalibrations on that window using the **Change X-Calibration of Acquisition** dialog box. If you save (under its previous filename) data that has been recalibrated in pixels, you will lose any previously saved calibration.

## 4.2.3 - Center Wavelength / Center of Raman Shift

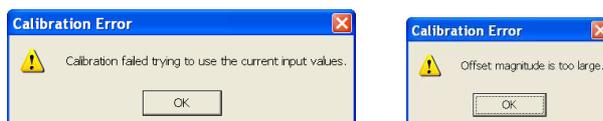
The system allows you to adjust your spectrograph so that light of a chosen **Wavelength** or a chosen **Raman Shift** falls on the center of the CCD-chip.

These are referred to as the **Center Wavelength** and the **Center of Raman Shift** respectively.

If you have chosen **Wavelength** as your X-Axis Label, enter the **Center Wavelength** in the text box provided on the Spectrograph X-Calibration dialog box. If you have chosen **Raman Shift** as your X-Axis Label enter the **Center of Raman Shift** in the text box.

In each instance, the value is expressed in the units you selected previously above.

If you enter too large or too small a value an **Error** dialog box appears, e.g.:



### 4.2.3.1 - Note on Raman Shift

The **Raman Shift** is calculated as follows:

If **scatter** is the wavelength of the Raman scattered light in nanometers and **laser** is the wavelength of the incident laser light in nanometers, then the Raman Shift in  $\text{cm}^{-1}$  (i.e. **rs**) is calculated as follows:  $rs = 10^7 \times [(\text{scatter} - \text{laser}) / (\text{scatter} \times \text{laser})]$ .

Thus, if **scatter** < **laser**, a negative Raman Shift (**anti-Stokes transition**) will result.

If **scatter** > **laser**, a positive Raman Shift (**Stokes transition**) will result.

Positive and negative values for Raman Shift may thus appear on the x-axis of a data window that is calibrated for Raman Shift, and may be used in the calibration process itself.

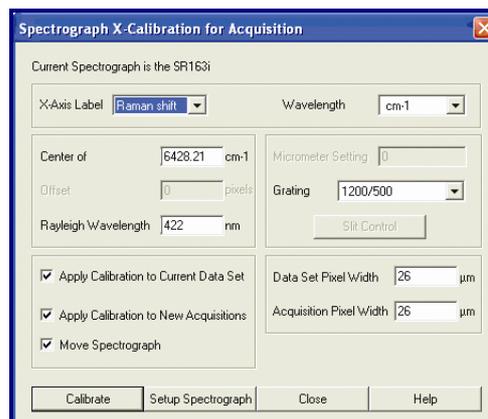
## 4.2.4 - Offset

By entering a value in the **Offset** text box of the Spectrograph X-Calibration dialog box you can compensate for small misalignments of the detector or the wavelength drive in your spectrograph. A positive value will cause the x-axis of the data window to move to the right (relative to the trace) by the corresponding number of pixels. A negative value will cause the x-axis to move to the left.

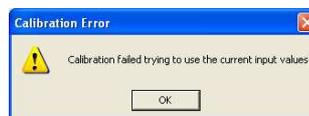
**NOTE:** To assess the accuracy of any calibration you have performed, you will need a calibration spectral line source, such as a helium neon laser or a mercury vapor lamp. Ideally, set the spectrograph to one of the prominent spectral lines, take a scan, and use the cursor on the data window to determine any offset (in pixels) of the line from its true wavelength.

## 4.2.5 - Rayleigh Wavelength

If you have selected **Raman Shift** as your X-Axis Label, you must enter a value in nanometers for the **Rayleigh Wavelength**. In Raman Spectroscopy the Rayleigh Wavelength is that element of a spectrum line (in scattered radiation) whose wavelength is equal to that of the incident radiation (i.e. the laser wavelength) and is a product of ordinary or Rayleigh scattering.



A **Calibration Error** message will appear if you attempt to perform a calibration without having entered a valid Rayleigh Wavelength, e.g.:



**4.2.6 - Micrometer Setting with Raman Shift**

For certain non-motorized spectrographs, the system will calculate a **Micrometer Setting** that corresponds to the **Grating** and the **Center Wavelength / Center of Raman Shift** you have chosen. The Micrometer Setting allows you to manually adjust the angle of the diffraction grating (by means of the micrometer on the spectrograph housing), so that light of the wavelength / Raman shift of your choice falls on the centre of the CCD-chip.

The Micrometer Setting appears in a text box on the Spectrograph X-Calibration dialog box. You should use this value to manually set the micrometer on the spectrograph.

**NOTE: If you choose to enter a micrometer setting, the system will calculate a value for the center wavelength / center of Raman shift, and vice versa. You need enter only one of the two values.**

Because Raman shift does not correlate linearly with wavelength (or pixel positions), the center column of pixels on the CCD-chip (e.g. column 512 on a chip of 1024 pixels) is likely to be represented off-center on the x-axis of a data window linearly calibrated for Raman shift. Column and where appropriate, row number, are expressed in the form **[x,y]** on the status bar along the bottom edge of the data window.

**NOTE: If you choose Raman shift as the X-Axis label, the center wavelength text box is relabeled center of raman shift.**

**4.2.7 - Grating**

From the scrollable drop-down list select the specification of the diffraction grating you are currently using. **Grating** specifications are shown as a line density followed by (where applicable) a blaze wavelength.

**4.2.8 - Close**

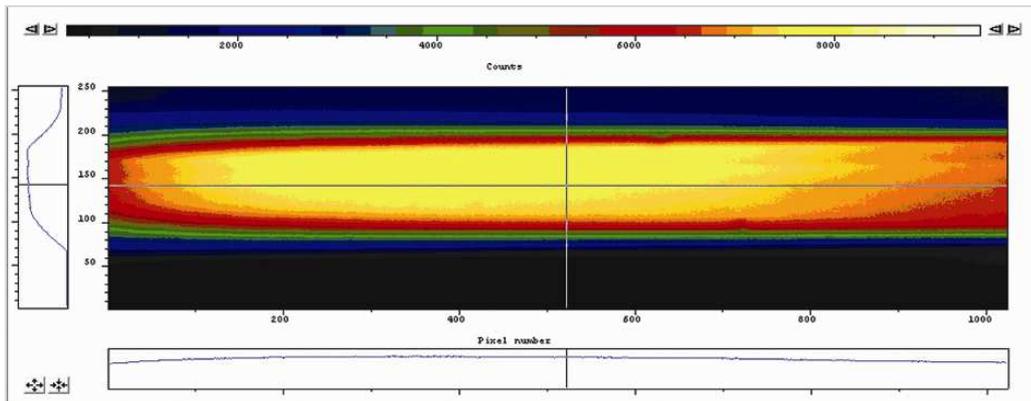
To exit the Spectrograph X-Calibration dialog box, click Close.

**NOTE: The details you supply regarding your spectrograph, including any retrieved data, will subsequently appear by default whenever you open the Spectrograph X-Calibration dialog box. You can change them whenever you choose.**

**4.3 - ADJUSTING THE DETECTOR WITH A CONTINUOUS WAVE (CW) SOURCE**

In order to optimal performance, we recommend you carry out the following procedure:

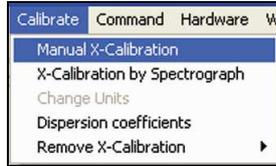
1. Fit a suitable input accessory (e.g. slit or fiber interface)
2. Loosely attach detector to output flange
3. Couple a suitable **CW** light source to the input port
4. Set the display mode in **SOLIS** to **Imaging**, with appropriate timing
5. Select **Large Cursor** from the **Display, Preferences** dropdown menu and place it in the middle of the image
6. Check that the signal trace lines up with the cross-hairs (adjusting the detector if required) e.g.:



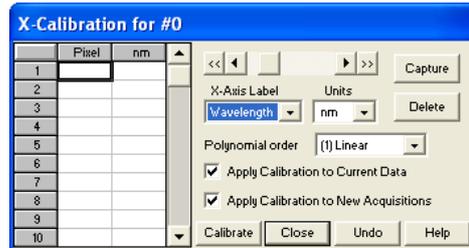
When the image is correctly aligned, secure the holding screws.

**4.4 - MANUAL X-CALIBRATION**

Using newly acquired or previously stored data, select **Manual X-Calibration** from the **Calibrate** menu:



The **Manual X-Calibration** dialog box appears, e.g.:



The number (**#n**) of the data window (or **#0** in the case of an Acquisition Window) appears on the title bar of the dialog box.

## 4.4.1 - Supplying Calibration Details

To manually calibrate a data window, first use the drop-down lists on the Manual X-Calibration dialog box to choose the **label** and the **units** you wish to use for the x-axis. The available labels and units are shown here:

X-AXIS LABEL	UNITS
Wavelength	nm, $\mu\text{m}$ , $\text{cm}^{-1}$ , eV
Raman Shift	$\text{cm}^{-1}$
Position	$\mu\text{m}$ , mm, cm, $\mu\text{i(nches)}$ , in(ches)
Time	ms, secs
Pixel	pixels

Your chosen unit will appear on the top of the right-hand column of the two columns to the left of the Manual X-Calibration dialog box.

Another drop-down list allows you to choose a **polynomial order** for your calibration. The following polynomial options are available:

POLYNOMIAL ORDER	DESCRIPTION
Linear	The linear fit is best for situations where only 2 or 3 spectral features can be identified.
Quadratic	A quadratic polynomial produces the best calibration fit if the known spectral features are located near the centre of the CCD sensor.
Cubic	A cubic polynomial produces the best calibration fit if the known spectral features are evenly distributed across the CCD sensor.

To perform the calibration:

1. Place the cross-hairs on a feature which you know to have a particular x-axis value and click **Capture**. If you wish to remove a point that you had previously selected, click **Delete**.
2. The pixel number will appear in the left-hand column. Against it, in the right-hand column, enter a value.

Repeat steps **1 & 2** above for at least one other point. However, to achieve a good quality calibration you should choose a polynomial order fit commensurate with the spread of known spectral features across your sensor.

## 4.4.2 - Applying Calibration

Two check boxes on the Manual X-Calibration dialog box allow you to choose how the system should act upon the calibration details you have provided. You may select either or both of the following options:

- **Apply Calibration to Current Data:** allows you to change the x-axis calibration on an active data window whose filename (or #0 in the case of an Acquisition Window) appears on the title bar of the Manual X-Calibration dialog box.

**Apply Calibration to New Acquisitions:** the calibration details you have supplied in the Manual X-Calibration dialog box will be applied to any subsequent data acquisitions.

## 4.4.3 - Calibrate

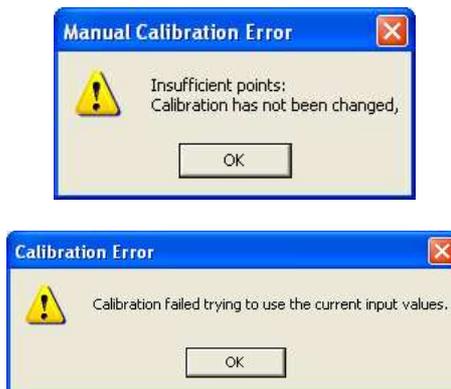
Depending on the selections made using the check boxes on the Manual X-Calibration dialog box, clicking the **Calibrate** button will apply calibration to the active data window and/or to future data acquisitions.

## 4.4.4 - When Manual X-Calibration goes wrong

In the event that **Manual X-Calibration** fails, it typically does so for one of two reasons:

- Data that you are attempting to calibrate are **non-monotonic** (for example, a wavelength that should correspond to a single pixel value has several pixel values)
- You have identified **too few points** (i.e. 0 or 1) for the system to perform a calibration.

The system displays one of the following dialog boxes depending on the nature of the error.:

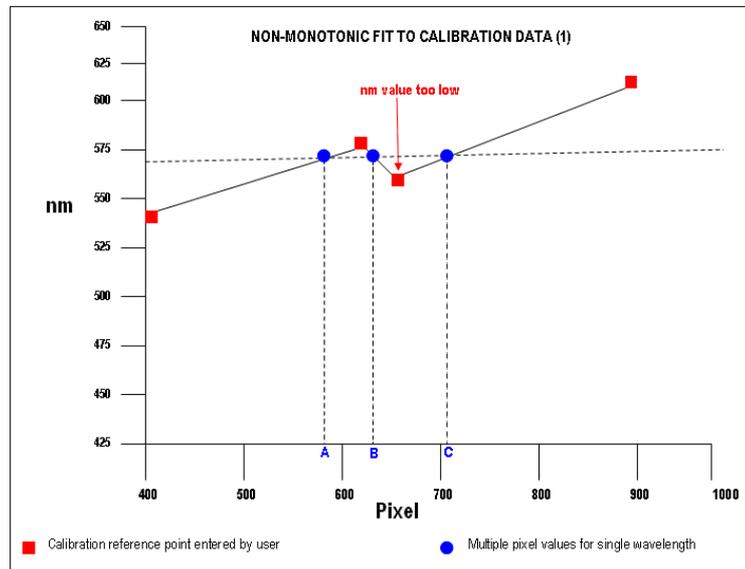


## 4.4.4.1 - Data are Non-Monotonic

Your data may be “**Non-Monotonic**” if you have entered an incorrect value for one or more points on your data trace. An instance of grossly inaccurate manual calibration is shown here:

	953	nm
1	457	546.1
2	690	577
3	706	550
4	953	612
5		
6		
7		
8		
9		
10		

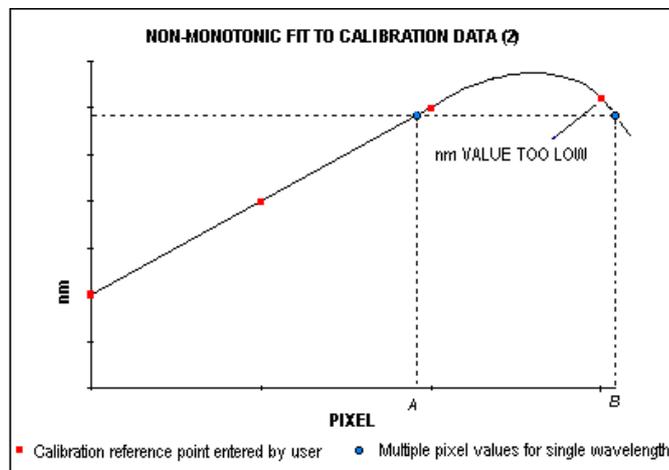
From Pixel 706 to Pixel 953 the user has indicated a fall in wavelength, despite the preceding rise in pixel 690. In such a case, an illegal non-monotonic calibration (as shown on the graph below) results. The squares indicate points entered by a user, pixel values *A*, *B* and *C* illustrate the non-monotonicity of a sample wavelength of around 570 nm (i.e. three different pixel values for a single wavelength).



However, a non-monotonic calibration may come about even in cases where your data are not as grossly inaccurate as those shown in the example above. A non-monotonic calibration sometimes results if you attempt to calibrate points that are very close together on your trace, even if, for example, you are entering rising wavelength values against rising pixel values.

In its background processing, the system models the calibration data (the user-supplied reference points) as a cubic polynomial. Inaccurate values mapped to pixels that are close together may cause the system to model the calibration data as shown in the following graph.

Again certain (wavelength) values are non-monotonic relative to pixel value (see pixel values *A* and *B*, for example). The squares on the graph indicate points entered by the user, the rightmost point being at slightly too low a wavelength value.



## 4.4.4.2 - Too few points

A calibration error will also occur if you have entered no data points, or only one data point, in the Manual X-Calibration dialog box. As general rule to obtain a good quality calibration, use more than five reference points, at regular intervals, across the full width of the CCD sensor.

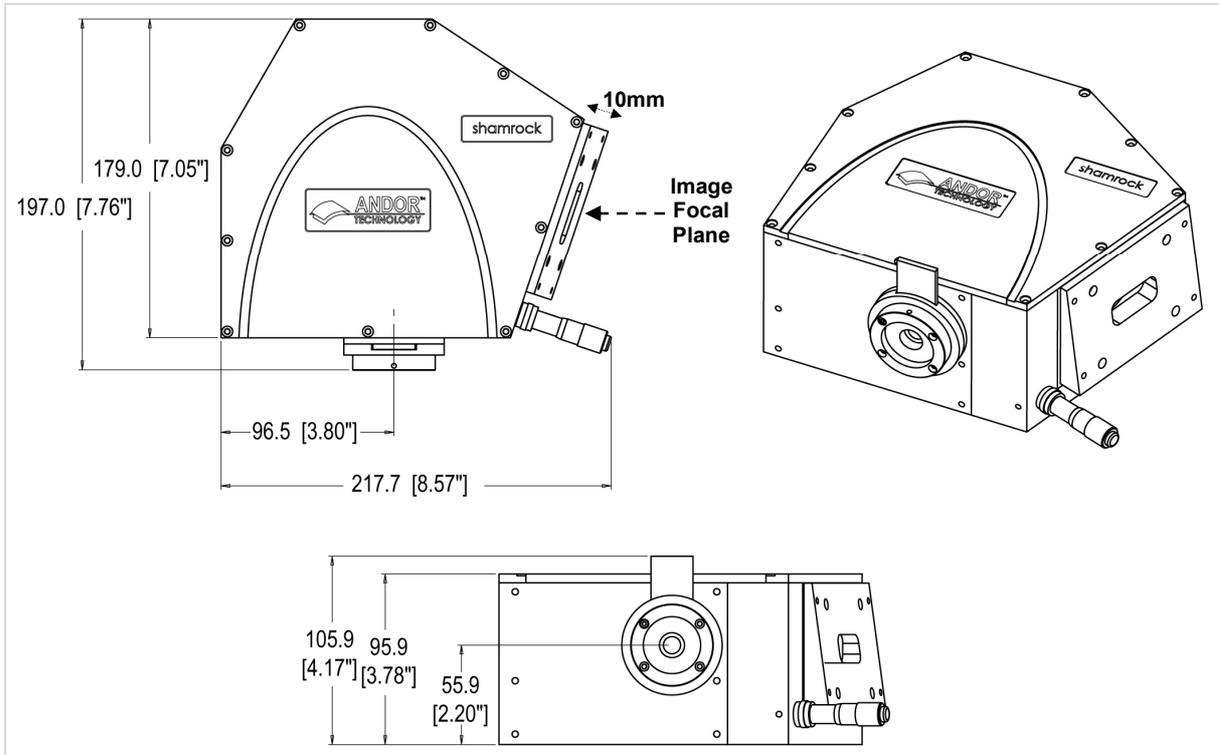
## 4.4.5 - Undo

Click the **Undo** button to exit the Manual X-Calibration dialog box and to undo any calibrations that you have performed since entering the dialog box.

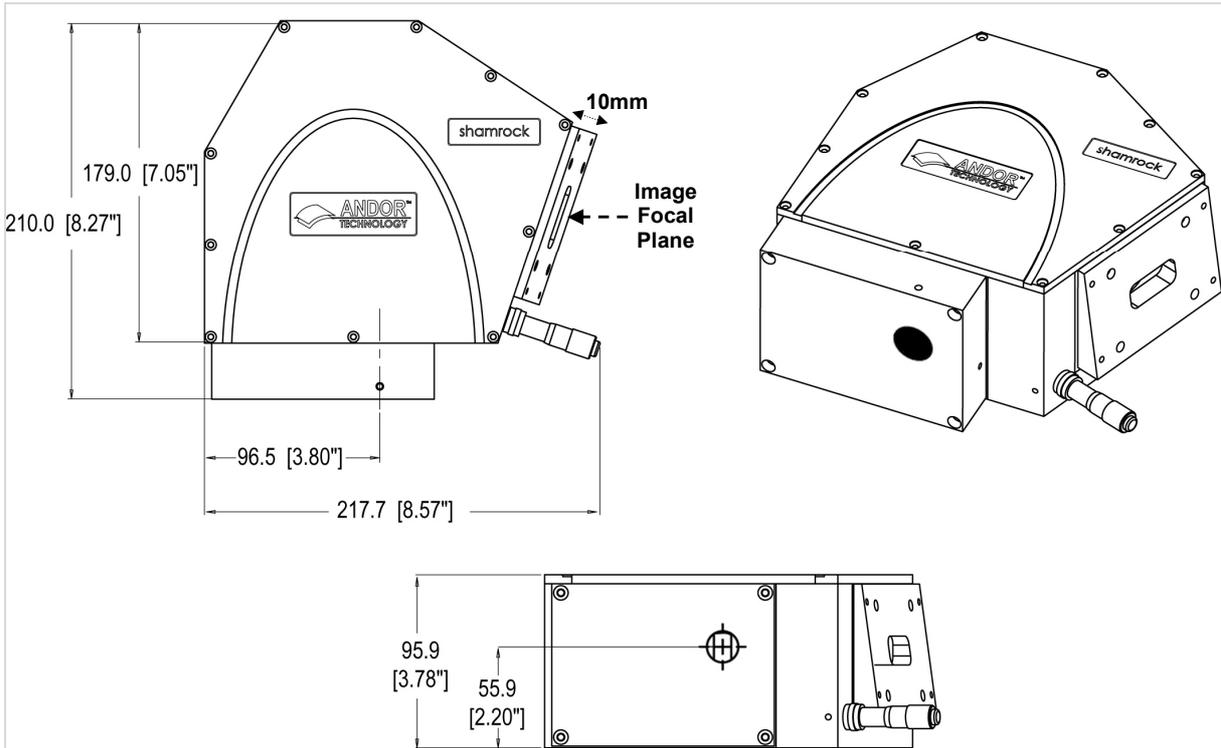
## 4.4.6 - Close

Click the **Close** button to exit the Manual X-Calibration dialog box.

**APPENDIX**  
**A1.1 - MECHANICAL DRAWINGS**  
**A1.1.1 - Spectral Mode**



**A1.1.2 - Imaging Mode**



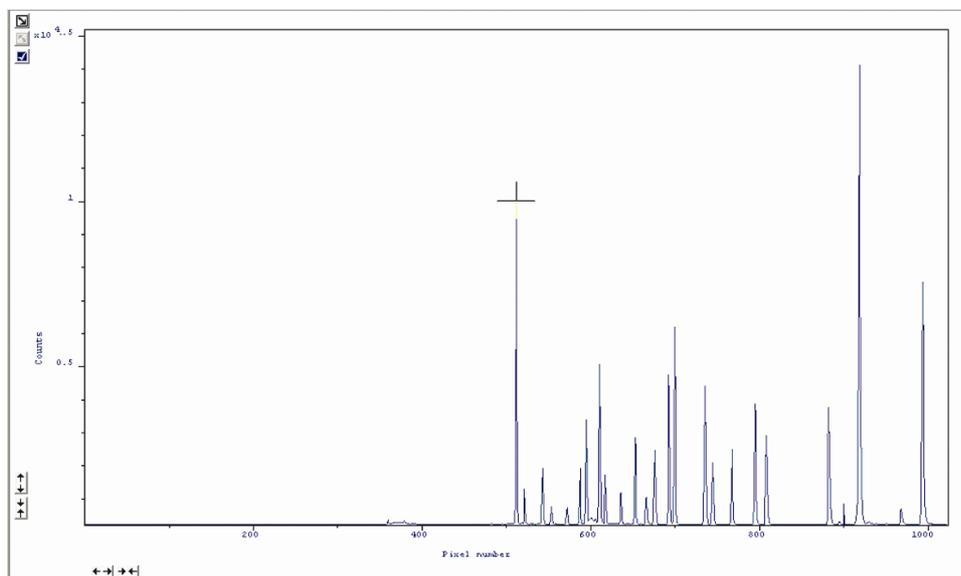
**A1.2 - TABLE OF SPECTRUM REFERENCES**

Spectral reference lines useful for Wavelength Calibration:

Wavelength (µm)	Light source
253.7	UV
365.0	UV
404.7	Violet (Faint)
407.8	Violet
507.3	2 <sup>nd</sup> Order UV line
546.1	Visible: Green
632.8	Visible: Helium-Neon Laser
730.0	2 <sup>nd</sup> Order UV line
760.9	3 <sup>rd</sup> Order UV line
809.4	2 <sup>nd</sup> Order – Violet (dim)
871.6	2 <sup>nd</sup> Order - Blue

**A1.3 - EXAMPLE SPECTRA**

Here is an example of spectra captured from a Neon-Argon source using a 25mm slit and 1200l/mm grating:



## A1.4 - TERMS &amp; CONDITIONS

In these conditions:

'Buyer' means the person who accepts a quotation of the seller for the sale of the goods or whose order for the goods is accepted by the seller.

'Goods' means the goods (including any instalment of the goods or any parts for them) which the seller is to supply in accordance with these conditions.

'Seller' means Andor Technology plc.

'conditions' means the standard terms and conditions of sale set out in this document and (unless the context otherwise requires) includes any special terms and conditions agreed in writing between the buyer and seller.

'Contract' means the contract for the purchase and sale of the goods.

'Writing' includes telex, cable, facsimile transmission and comparable means of communication.

2. Any reference in these conditions to any provision of a statute shall be construed as a reference to that provision as amended, re-enacted or extended at the relevant time.
3. The headings in these conditions are for convenience only and shall not affect their interpretation.

**A1.5 - WARRANTIES & LIABILITY**

1. Subject to these conditions set out below, the seller warrants that the goods will correspond with their specification at the time of delivery and will be free from defects in material and workmanship for a period of 12 months from the date of delivery.
2. The above warranty is given by the seller subject to the following conditions:
  - 2.1 The seller shall be under no liability in respect of any defect in the goods arising from any drawing, design or specifications supplied by the buyer;
  - 2.2 The seller shall be under no liability in respect of any defect arising from fair wear and tear, wilful damage, negligence, abnormal working conditions, failure to follow the seller's instructions (whether oral or in writing), misuse or alteration or repair of the goods without the seller's approval;
  - 2.3 The seller shall be under no liability under the above warranty (or other warranty, condition or guarantee) if the total price for the goods has not been paid by the due date for payment;
  - 2.4 The above warranty does not extend to parts, material or equipment not manufactured by the seller, in respect of which the buyer shall only be entitled to the benefit of any such warranty or guarantee as is given by the manufacturer to the seller.
3. Subject as expressly provided in these conditions, and except where the goods are sold to a person dealing as a consumer (within the meaning of the unfair contract terms act 1977), all warranties, conditions or other terms implied by statute or common law are excluded to the fullest extent permitted by law.
4. Any claim by the buyer which is based on any defect in the quality or condition of the goods or their failure to correspond with specification shall (whether or not delivery is refused by the buyer) be notified in writing to the seller within 7 days from the date of delivery or (where the defect or failure was not apparent on reasonable inspection) discovery of the defect or failure. If delivery is not refused, and the buyer does not notify the seller accordingly, the buyer shall not be entitled to reject the goods and the seller shall have no liability for such defect or failure, and the buyer shall be bound to pay the price as if the goods had been delivered in accordance with the contract. In no event shall the buyer be entitled to reject the goods on the basis of any defect or failure which is so slight that it would be unreasonable for him to reject them.

5. Where any valid claim in respect of the goods which is based on any defect in the quality or condition of the goods or their failure to meet specification is notified to the seller in accordance with these conditions, the seller shall be entitled to replace the goods (or the part in question) free of charge or, at the seller's sole discretion, refund to the buyer the price of the goods (or a proportionate part of the price), but the seller shall have no further liability to the buyer.

6. Except in respect of death or personal injury caused by the seller's negligence, the seller shall not be liable to the buyer by reason of any representation (unless fraudulent), or any implied warranty, condition or other term, or any duty at common law, or under the express terms of the contract, for any indirect, special or consequential loss or damage (whether for loss of profit or otherwise), costs, expenses or other claims for compensation whatsoever (whether caused by the negligence of the seller, its employees or against otherwise) which arise out of or in connection with the supply of the goods, or their use or resale by the buyer and the entire liability of the seller under or in connection with the contract shall not exceed the price of the goods, except as expressly provided in these conditions.

7. The seller shall not be liable to the buyer or be deemed to be in breach of the contract by reason of any delay in performing, or any failure to perform, any of the seller's obligations in relation to the goods, if the delay or failure was due to any cause beyond the seller's reasonable control. without prejudice to the generality of the foregoing, the following shall be regarded as causes beyond the seller's reasonable control:

7.1 Act of god, explosion, flood, tempest, fire or accident;

7.2 War or threat of war, sabotage, insurrection, civil disturbance or requisition;

7.3 Acts, restrictions, regulations, bye-laws, prohibitions or measures of any kind on the part of any governmental, parliamentary or local authority;

7.4 Import or export regulations or embargoes;

7.5 Strikes, lock-outs or other industrial actions or trade disputes (whether involving employees of the seller or of third party);

7.6 Difficulties in obtaining raw materials, labour, fuel, parts or machinery;

7.7 Power failure or breakdown in machinery.