Installation and Operation Manual

Arcspectro FT Rocket Fourier-Transform Spectrometers

Software Version 3.2

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Content

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The effective date of this warranty shall begin on the date of shipment/date of invoice, whichever is later. Products are warranted to be free from defects in materials and workmanship for parts and labor for 1 year with the exceptions indicated below:

Limitations

Products are warranted to be free from defects in materials and workmanship for parts and labor for 1 year with the following exceptions:

- Any components of the system that are in direct contact with corrosive materials are warranted to be free from defects in materials and workmanship at time of delivery but cannot be further warranted due to the unknown nature of the use of the product.
- Consumable items such as lamps, cuvettes and optical filters are excluded from this warranty. If a lamp undergoes a catastrophic failure (e.g., no light at all) within 90 days of shipment from the factory, it will be replaced at no charge.
- Loss, damage, or defects resulting from transportation to the Buyer's facility, improper or inadequate maintenance by Buyer, software or interfaces supplied by the buyer, unauthorized modification or operation outside the environmental specifications for the instrument, use by unauthorized or untrained personnel or improper site maintenance or preparation.
- The sole and exclusive warranty applicable to software and firmware products provided by Seller for use with a processor internal or external to the Product will be as follows: Seller warrants that such software and firmware will conform to Seller's program manuals or other publicly available documentation made available by Seller current at the time of shipment to Buyer when properly installed on that processor, provided however that Seller does not warrant the operation of the processor or software or firmware will be uninterrupted or error free.
- Products that have been altered or repaired by individuals other than Arcoptix personnel or its duly authorized representatives, unless the alteration or repair has been performed by an authorized factory trained service technician in accordance with written procedures supplied by Arcoptix.
- Products that have been subject to misuse, neglect, accident, or improper installation.

The warranty herein applies only to Products within the country of original delivery. Products transferred outside the country of original delivery, either by the Seller at the direction of the Buyer or by Buyer's actions subsequent to delivery, may be subject to additional charges prior to warranty repair or replacement of such Products based on the actual location of such Products and Seller's warranty and/or service surcharges for such location(s).

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Repaired products are warranted for 90 days with the above exceptions.

CHAPTER 1 Introduction

1.1 Product description

The ARCspectro FT ROCKET is a family of near-infrared (NIR) and mid-infrared (MIR) scanning Fourier-transform (FT) spectrometers. They are high precision opto-mechanical devices combining optics, micromechanical actuation and electronics. At the heart of the FT ROCKET spectrometers is a white-light interferometer, whose motion is measured with extreme precision by a solid-state reference laser. Dedicated optical components bring the light through the interferometer mirrors to the detector.

The spectrometers are packaged in a friendly housing, including all necessary electronics with the A/D converter and the USB data transfer, shown in Figure 1-1:

Figure 1-1 The Fourier-transform spectrometer FT-NIR Rocket. One distinguishes the input connector for the optical fiber, bringing the light into the spectrometer. Data transfer to the computer and power supply (for non-cooled detectors) are done by the USB connection.

The ARCspectro FT ROCKET family of fibered spectrometers includes :

- **FT-NIR ROCKET:** covers a wavelength range of 0.9-2.6 micrometers with InGaAs photodiodes (uncooled or thermoelectrically cooled versions). It can be coupled via low –OH content NIR fibersand many commerciall available NIR sampling accessories.
- **FT-MIR ROCKET**: covers a wavelength range of 2.0-6.0 micrometers with thermoelectrically cooled MCT detectors. It can be used with commercially available Chalcogenide MIR fibers and MIR sampling accessories.
- **FT-IR ROCKET (OEM)** ARCoptix also commercializes free-space (non-fibered) versions of the FT Rocket for OEM applications, with wavelength ranges covering up to 2-12 micrometers using thermoelectrically cooled MCT detectors (wave-number range 830-5000 cm^{-1}). Please contact ARCoptix for further information.
- **GASEX and GASEX PORTA** MIR spectrometers coupled to a Gas cell designed for gas mixtures analysis.

1.2 Principle of operation

The heart of the FT-Rocket is **dual** retro-reflector interferometer, schematized in Figure 1-2. The two retro-reflectors are solidary to a common swinging arm, which rotates to create an optical path difference in the two arms of the interferometer.

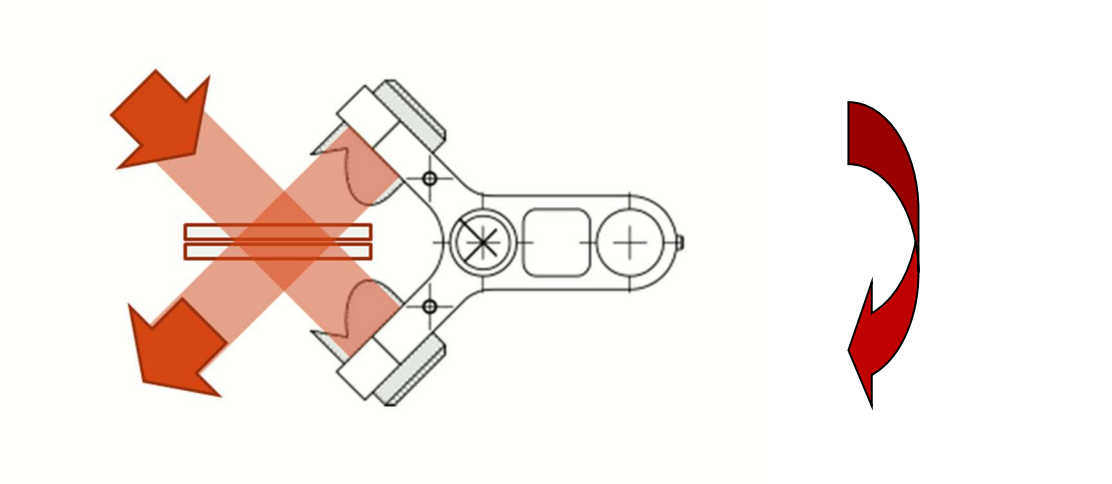


Figure 1-2 - The principle of operation of the FT Rocket interferometer

This type of design is called a **permanently aligned** interferometer, as the alignment of the system know to be the most rubust against vibrations and temperature drifts. It never has to be realigned.

The swinging arm of the interferometer rotates on **wear-free flexture system**, making this mechanical system extremely robust and long-lifed.

When monochromatic light enters an ideal interferometer, the signal recorded at the detectors has the form:

$$I(\delta) = I_0 R_{BS} T_{BS} \left[1 + \mathrm{m} \cos \frac{2\pi}{\lambda} \delta\right]$$

where I_0 is the intensity of the light entering the interferometer, R_{BS} and T_{BS} are the beam splitter reflectivity and transmission, m is called the modulation coefficient (which is close to 1). It is a sinusoidal function of the optical path difference δ, whose period is dependent on the wavelength of light.

The AC component of $I(\delta)$ is called the *interferogram*. Very basically, if the light entering the interferometer is composed by a continuous spectrum $S(\upsilon)$, where $\upsilon = \frac{1}{\lambda}$ is called the light wave number, Then the recorded interferogram is the integral over all wave numbers υ:

$$I^{AC}(\delta) = \int_{-\infty}^{+\infty} S(\upsilon) \mathrm{m} \cos(2\pi\upsilon\delta) d\lambda$$

The recorded interferogram $I^{AC}(\delta)$ contains all information about the spectral composition $S(\lambda)$ of the incoming light, which can be extracted by using mathematical operation called a *Fourier transformation*:

$$S(\upsilon) = \int_{-\infty}^{+\infty} I^{AC}(\delta)\ \mathrm{m}\cos(2\pi\upsilon\delta)d\delta$$

1.3 System requirements

The spectrometer connects to a notebook or desktop PC via a USB 2.0 port. Spectrometers also require an additional external 12V DC power supply. The optics, mechanics and electronics share the same single housing.

The Arcspectro FT ROCKET can connect via the USB 2.0 (or USB 3.0) port to any PC that uses a Windows 64 bits 7 or 10 operating system and has the spectrometer operating software installed and configured for use with your Arcspectro FT ROCKET.

An EEPROM memory chip in each Arcspectro FT ROCKET spectrometer contains calibration parameters and the serial number unique to each spectrometer. The operating software reads these values from the spectrometer.

The Arcspectro FT Rocket has two or three input connectors, depending on the version:

- one FSMA receptacle which accepts a fiber optic cable with a standard SMA-905 connector
- one USB port which connects to a USB host (computer) via a standard USB cable
- one connector for the external for a 12V power supply
- Optionally on Gasex porta devices an ethernet connector.

1.4 Items Included with the shipment

Important information and documentation accompany your Arcspectro FT ROCKET spectrometer upon shipment. This includes:

- **Software and manual USB key** – Each spectrometer order comes with Arcoptix software CD. This disc contains all Arcoptix software and manuals for software operation. Documentation is provided in Portable Document Format (PDF). You need Adobe Acrobat Reader to view these files.
- **USB cable**
- **12V DC Power supply** (not with USB-powered spectrometer versions)

CHAPTER 2 Installing the Arcspectro FT spectrometer

2.1 General information

Important: You must install the operating software application prior to connecting the Arcspectro FT ROCKET spectrometer to the PC.

The Arcspectro spectrometer operating software installs the drivers required for Windows to communicate with the Arcspectro FT ROCKET. If you do not install the software first, the system might not properly recognize the Arcspectro FT ROCKET.

Follow the steps in this section to interface the Arcspectro FT ROCKET Spectrometer via the USB port to a desktop or notebook PC.

To connect the FT ROCKET Spectrometer to a PC via the USB port, the PC must be running windows 7/10 64 bits operating system. *You must have administrator privileges in order to run the installation package*.

2.2 Software Installation

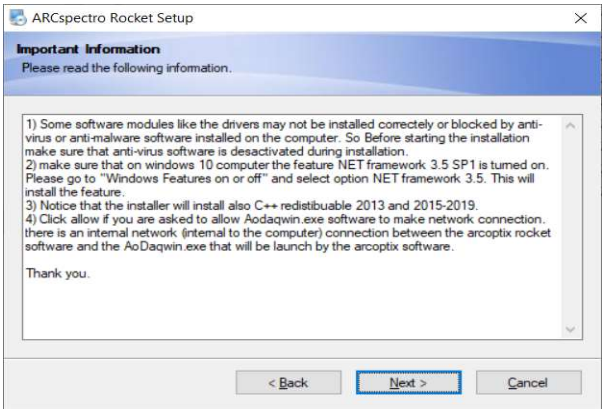
The setup is a semi-automated procedure including the following installation stages:

- Detection and installation of eventual missing packages like 2013 or 2015-2019 C++ redistributable packages.
- Installation of the main software
- Installation of the device drivers
- Connection of the device to the computer.

2.2.1 Detailed installation steps

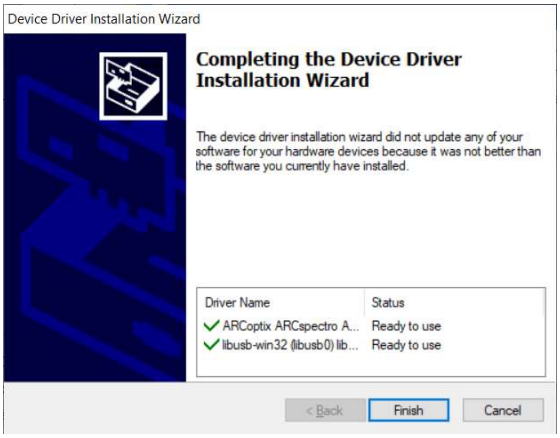
1. Disable or switch off eventual anti-virus or anti-malware application that may bloc the installation.
2. Run the ARCspectroRocket 3.2.0 Installation Package.exe

3. The installer will verify if the requested versions of the .Net Framework and c++ redistributable 2015-2019 64 bits are already installed. Following message will be showed:



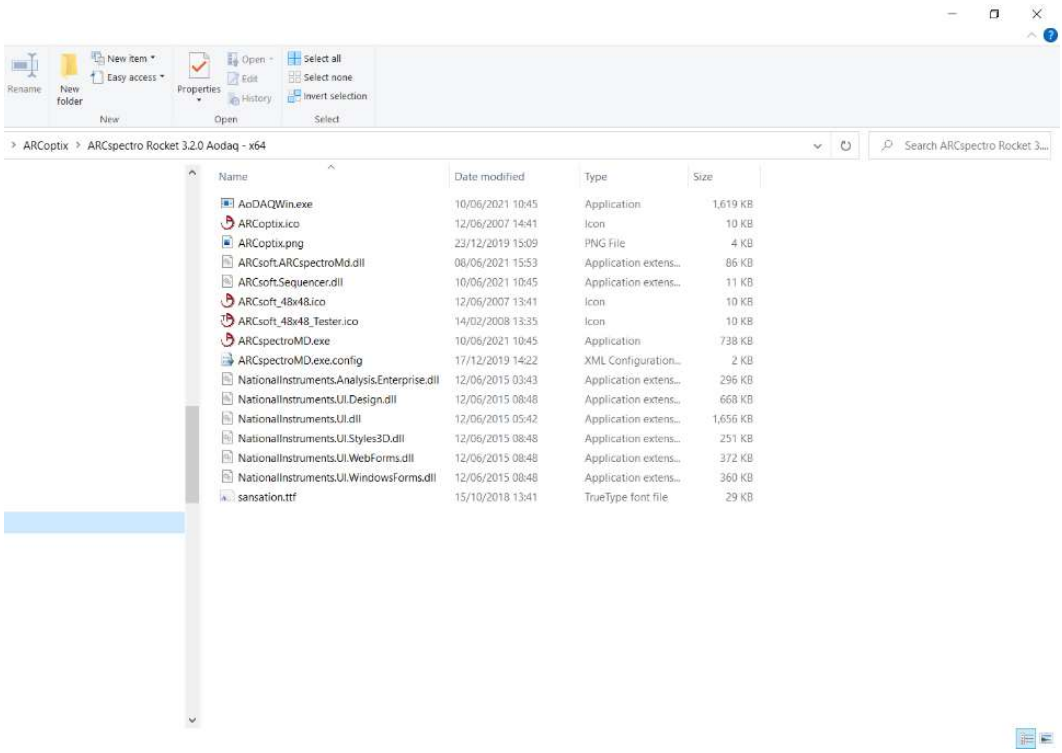
If not, the installer will install the redistributable C++. However, it will not be able to install missing .NET libraries.

4. Follow the installations steps
5. At the end of the installation device driver will be installed libusb-win 32



6. Software in now installed
7. Once the software and drivers are installed you may check in the device manager of windows if the Gasex is correctly recognize by windows (if you connect the USB to the computer (and switch on the device). It should be recognized as a libusb-win32 device.

   you can launch the application called **ARCspectroMD.exe** directly in the start menu of windows or via the Explorer in the program Files / Arcoptix folder as shown below



2.3 Hardware installation details

2.3.1 USB connection

The FT Rocket operates via a USB 2.0 or higher connection. You need to connect the spectrometer to your PC using the USB cable supplied with the spectrometer.

2.3.2 Power supply connection

Connect the 12V power supply to the spectrometer.

2.3.3 Optical input

The standard connection for the spectrometer is a SMA-905 fiber port. Remove the blue cap and screw in you optical fiber.

On the FT-IR 2-12 (and some customized systems), the fiber coupler is external and removable. This is useful if you want to couple a free-space propagating beam into the spectrometer.

To remove the fiber coupler, you need to use a 2.5mm Allen key. Untightening the 2 screws on the fiber coupler diagonal will release the fiber coupler.

2.3.4 Purge gas connection

Some of the Arcoptix spectrometers are equipped with a descicant that filters out the water vapour and CO2 present in the interferometer. Since the spectrometer is not fully hermetic to gases from the outside (there is always some leakage), the descicant will saturate after a certain time (typically one year). The descicant is placed in a holder accesible from the top side of the spectrometer. If the descicant becomes saturated, water vapour and CO2 absorption lines will become more pronouced. To reduce the impact of those lines (that may interfer with gases the user wants to measure), it is recommended to repalce the descicant with a fresh one. For doing so, unscew the descicant cover (6 screws) and repalce it with the fresh the descicant (with the inscriptiions looking upwards) as showed in the picture. Finally close the holder again with the 6 screws. Notice that the descant saturates very quicly in an open environment (outside his plastic package or outside the desciant holder). The replacement operation has to be performed quickly (open the holder before openenin the desciant package). You will have to wait for a few hours before the level of water vapour significately reduces inside the interferometer (spectrometer). New Descicants can be ordered directly from Arcoptix.

2.4 Example measurement set-ups

2.4.1 Transmission measurements

In a setup for transmission/reflection, you will need:

- 2 fiber optical cables. Take optical fiber with large core diameter (i.e. 600 μm to 1000 μm) to assure optimal coupling condition and no loss of intensity.
- A sample, cuvette holder or probe
- A fiber-coupled light source

Light from the lamp is sent via optical fibers to a sample holder (or any other sampling accessory). The sample transmission is collected via fiber optic and sent to the spectrometer, as shown in Figure 2-1:

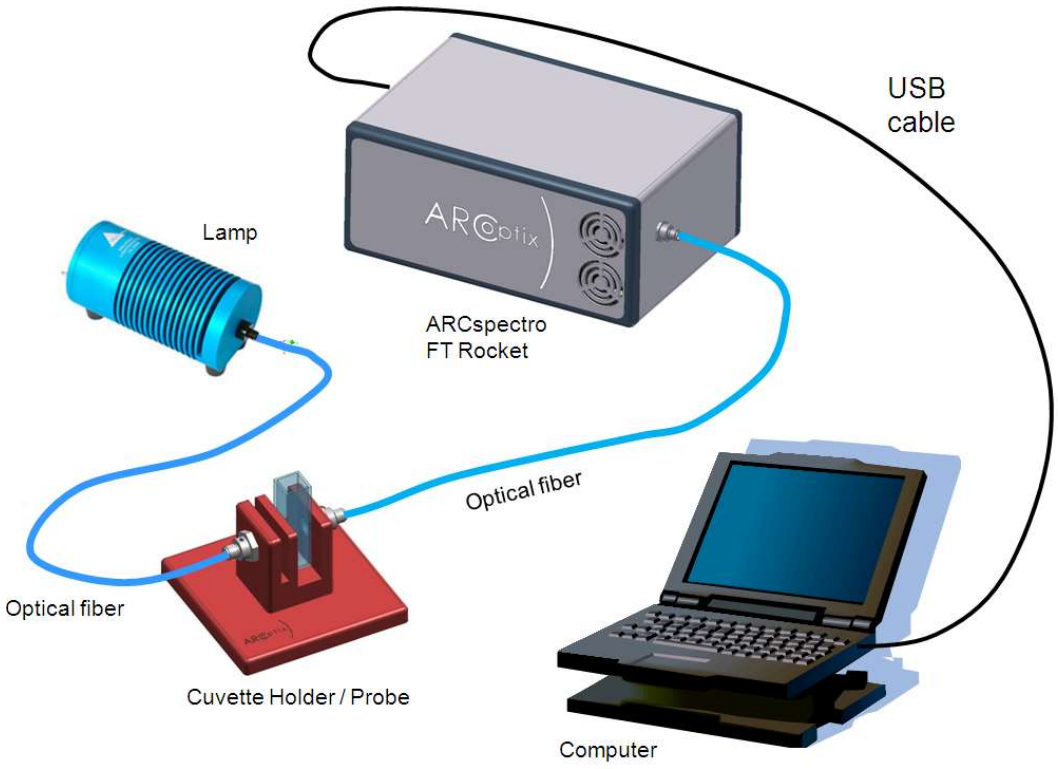


Figure 2-1 - Typical transmission measurement set-up

The following steps have to be performed to prepare for a measurement:

1. Connect the optical fiber to the lamp.
2. Connect optical fiber to the sample holder/probe for illumination. Note that there are sample holders and probes that have different connections for illumination and measurement.
3. Connect an optical fiber to the sample holder/probe and the spectrometer. It is recommended to use fibers with core diameters of at least than 500 μm.

4. Switch on the light source. If your light source has a shutter or an attenuator, ensure that these are open.
5. Connect the spectrometer via USB port to a PC with Arcspectro software already installed.
6. Start the Arcspectro program. This may take several seconds because of initialization and calibration that have to be loaded.
7. Start a single measurement by pressing the “Read” button 

.

The spectrometer and its software are now operational and allow you to use all features described in CHAPTER 3.

2.4.2 Reflection measurements

In similar way as transmission measurements, you can perform measurements in reflection. A possible setup is shown below in Figure 2-2. Reflection probes are available by different suppliers. These reflection probes usually contain several illumination fibers and one analysis fiber.

NOTE**:** Choose fibered optical probes with large core diameter fibers (e.g. 600µm) for optimal performance.

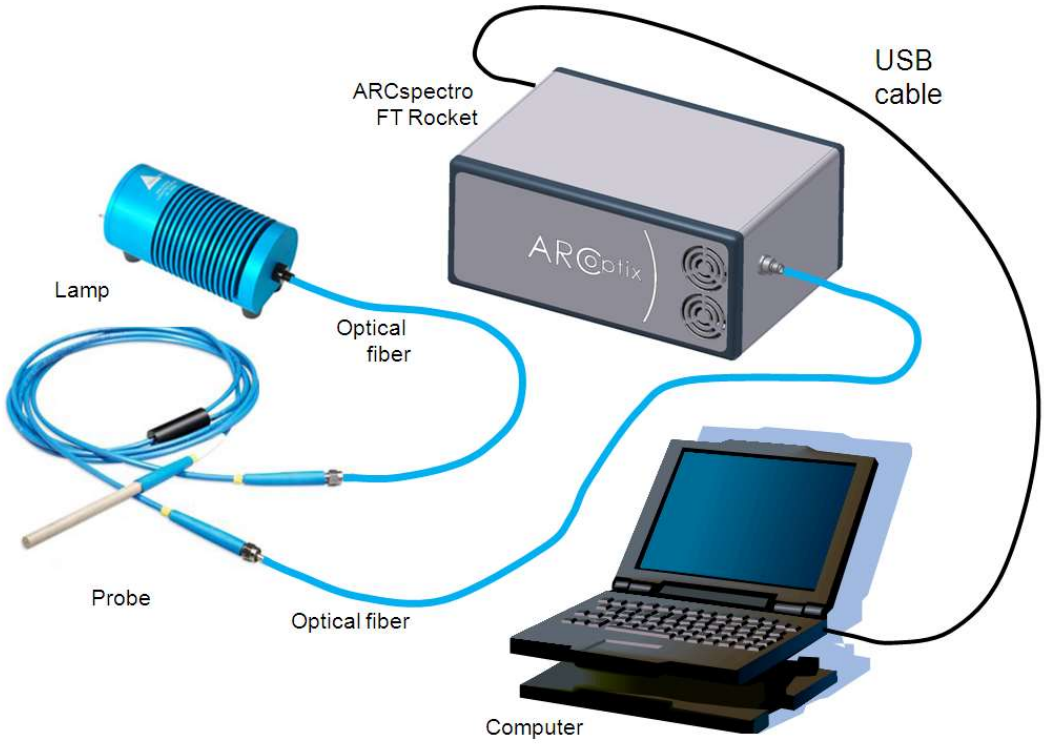


Figure 2-2 - Example of a reflection measurement setup employing a fibered reflection probe

2.4.3 Measurement of lasers – beam power limitations

Lasers can be measured by directly shining laser light into the spectrometer via an optical fiber of free-space entrance port.

Note that pulsed lasers (or pulsed sources in general) can only be measured if their repetition rate is faster that the FT Rocket interferometer modulation frequencies. Typically, only lasers with repetition rates above 25kHz can be measured. Please contact Arcoptix for further information.

Another important aspect is the **beam power limitation**, in order to avoid detector damage:

1) The CW, average or peak power of pulses longer then 1µs must not exceed 25mW

2) The peak power of pulses shorter than 1µs must not exceed 100W

3) For repeated irradiation with pulses shorter than 1 µs, the equivalent CW irradiation, i.e. average power over the pulse-to-pulse period should be less than the CW maximum power according to equation:

   (Equivalent CW radiation power) =
   (pulse peak power)*(pulse duration)*(repetition rate)

Failing to respect these beam power limitations will result in loss of warranty.

CHAPTER 3 Arcspectro FT software

3.1 General information

The Arcoptix FT ROCKET spectrometer is controlled by an application program. Spectral data is shown in the main window which is presented when the program is opened, presented in Figure 3-1:

Figure 3-1 – Graphical user interface of the Arcspectro application program.

Notice that once the program is started, the spectrometer is still not connected to the software and measurements cannot start directly. The user should first connect the spectrometer to the software with the connect to spectrometer button (see below).

It is important to understand that the software works with two executables:

1) A “server program” called AoDAQWin-exe that will be started in background on the computer. You may be requested (by windows security service) to authorize this executable to be started. This AODAQWin will be responsible to communicate with the spectrometer and also to make all the required signal processing (as for example the Fourier transform of the raw signal). This AoDaqwin executable will be started in background when connecting to the spectrometer (as explained below).
2) A “client program” as described in the figure above that is responsible to display (load, save, zoom,…) the measured spectra (preprocessed before by the AODAQWin executable that works in background.

Both programs described above will communicate with a (internal to the computer) TC-IP connection.

3.1.1 General Layout of the Window

In general, the program conforms to standard Windows conventions. For sake of brevity, features that are common to other windows programs (e.g. the dialog box for saving a spectrum is similar to that used for saving files in other programs) are not described. The window contains a menu bar, a toolbar and some other option bars that will be explained below. Above the measurement window the toolbar a line indicates important parameters such as the amplifier gain, resolution and the plot type.

3.2 Menu bars

3.2.1 Connect Spectrometer

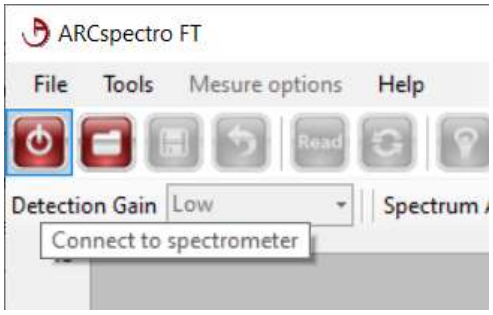
In order to connect the software to the spectrometer we need to setup a TCp-IP connection. This connection can be either

1) Internal to the computer via the address 127.0.0.1 (of the current computer)
2) External if the device is connected to the network or directely to the computer.

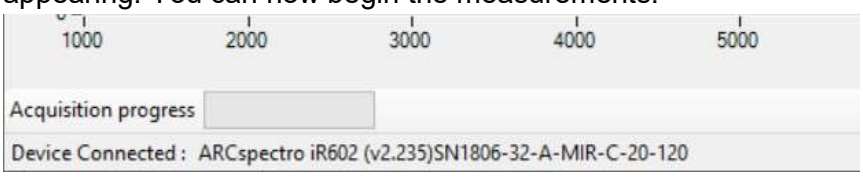
More info can be found in Annex at the end of the manual.

In case the spectrometer is connected via USB to the computer it is the internal connection to the computer that we will need to set-up.

1) Make sure that the spectrometer is connect to the computer and it is powered (12V).
2) Click connect to spectrometer

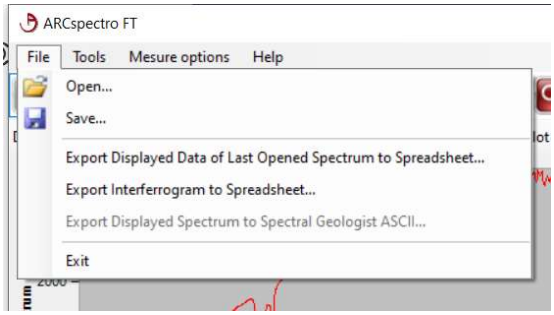


3) Click connect to USB Device (if it is usb connected). Notice that for a ethernet connected spectrometer either click search for device and it will give all the connected spectrometers visible on the internal network or enter directly the address of the device and click “connect to ethernet device”.
4) Wait for a moment. There will be a server application called AoDAQWin-exe that will be started in background on the computer. You may be requested to authorize this executable to be started. This AODAQWin will be responsible to communicate with the spectrometer and also to make all the required signal processing. This application may require important CPU resources and it is better not have many tasks running in parallel. Also notice that a message “Aodaq process is already running” may appear. Just click ok it this case. Waiting time maybe up to 1 minute.
5) Device connected you will see in the status bar the serial number of the device appearing. You can now begin the measurements.

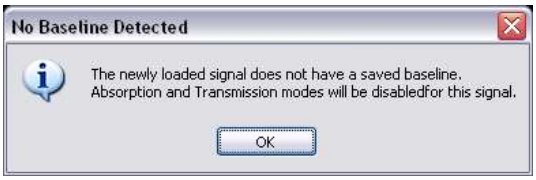


3.2.2 The File Menu

The *File* menu is used to access data storage and print functions.



Open… Presents a standard Windows dialog box to open data. Only binary files with the extension "*.arcspectro" are accepted. The loaded spectra will be shown in a different color on the screen. To delete the most recently loaded spectra use the return button. In the case that no baseline was measured with the original data the following message is shown.



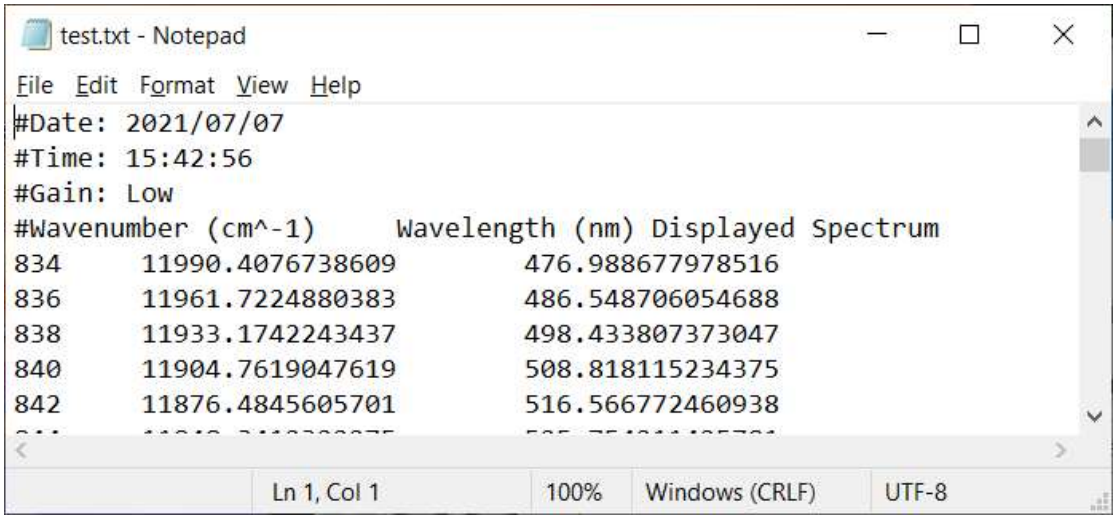
Save… Presents a standard Windows dialog box to save data. The file is saved as binary file and can be used for further data processing only with the ARCspectro software. It can be opened with the "Open" command. Only binary data can be saved. The extension is predefined as "*.arcspectro". All data will be saved containing all spectral information and a baseline.

A path and a filename have to be chosen and the data can be saved.

Export Displayed Spectrum to Spreadsheet…

Allows saving data in text spreadsheet format.

ONLY THE LAST RECORDER DATA WITH THE WAVELENGTHS RANGE AS SHOWN ON THE SCREEN WILL BE SAVED.
This includes functionalities like absorption and transmission. For example, if a spectra that shows absorption values in a narrow spectral range is exported you will only find these data in text file. The output format of the TXT file is shown here below:



Some indications about the measurements (3 first lines) and then 3 tab separated columns indicating: the wavenumber in cm-1, corresponding wavelength in nm and displayed spectrum in A.u.

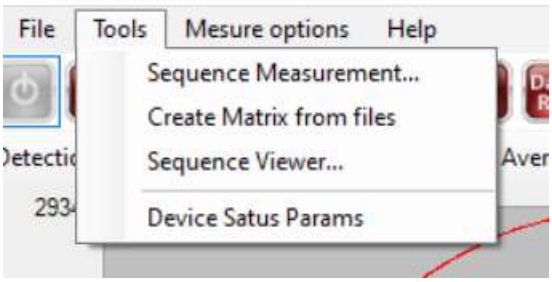
Exported files have no extension and can be opened with conventional programs (such as excel) for further processing.

Export Interferogram to Spreadsheet

Allows saving interferogram data in text spreadsheet format. Exported files have no extension and can be opened with conventional programs (such as excel) for further processing.

3.2.3 The Tools Menu

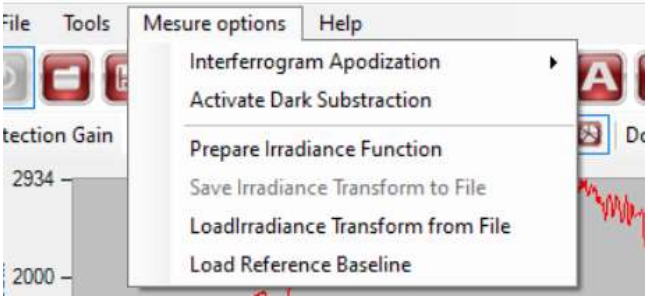
The Tools menu allows the user to access the Sequence measurement function. It gives the possibility to perform and analyze time series measurement. Two submenus are available. Sequence measurement and Sequence viewer. Please



Please refer to section 4.3.4 below in the manuel for further details about sequence measurements.

3.2.4 Measure options

These are advanced features, they are discussed in chapter 4.3 .



3.2.5 Help

Opens a window that provides information of the software version.


About ARCspectro FTIR
ARCoptix
Switzerland
ARCspectro Rocket
Version 3.2.0.0
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OK

3.3 Tools Bar

	**Open spectrum -** Presents a standard Windows dialog box to load already saved data that were saved as binary files. Several graphs can be loaded and shown in different colors on the screen.
	**Save Graphic -** Presents a standard Windows dialog box to save the active graph. Saved data represents all information with complete spectral range and baseline. Data are saved in binary format. For text format please EXPORT… data.
	**Remove last loaded spectrum -** Remove spectral data in the graph from the screen in the order of loading. The most recently loaded graph is removed first.
	**Read -** Starts a measurement. The button appears grey if the measurement is in progress.
	**Read continuously -** Collected spectra on a repetitive basis. Data collection is initiated upon selecting this option, and is terminated by pressing the button again.
	**Set baseline spectrum –** Sets the current measurement as baseline (reference) measurement and stores it for further treatment in local buffer. This operation has to be done before transmission or absorption measurements can be evaluated.
	**Set dark spectrum -** Sets the current measurement as dark (no light) measurement and stores it for further treatment in local buffer. This is useful when a constant background is present and needs to be removed. The dark substraction also has to be activated, see Chapter 4.3.2
	**Spectrum -** Sets the measurement modus in spectra mode and shows the raw spectral data recorded by the spectrometer.
	**Absorption -** Sets the measurement modus in absorption mode and shows the absorption relative to a white baseline measurement  that has to be done before.
	**Transmission -** Sets the measurement modus in transmission mode and shows the transmission relative to a baseline measurement  that has to be done before.
	**Zoom Tool -** Allows manual scaling by click and drag. Double click in the measurement window performs a autoscale 

	**Move graph -** On activating the graph can be moved laterally.
	**Autoscale -** Expands/contracts the vertical axis so that the minimum and maximum intensity and spectral range of the spectrum are at the minimum and maximum of the plot. Is also performed when the active window is double clicked.
	**Show interferogram -** Shows the raw data of the interferogram recorded by the device. The data are plotted against the optical path difference OPD.
	**Cursor toolbar -** Opens a courser toolbar at the bottom of the window. Please see the detailed explanation below.
	**Graphing options -** Opens a graphing options window at the right of the window. Please see the detailed explanation below.

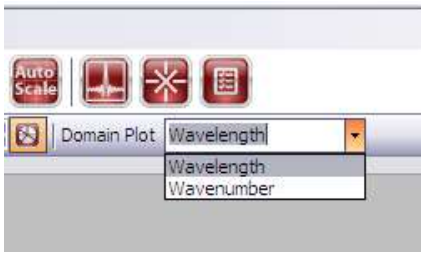
NOTE: If you are collecting data on a continuous basis or on a timed basis, some of the buttons are not active.

3.4 Options Bars

Detection gain Shows the amplification setting of the detector electronics. Four values can be chosen: **Low, Medium, High, Extreme**

Scans to average Several scans can be averaged using this option, e.g. in order to reduce measurement noise. The acquisition can be stopped by pressing the  button.

Domain plot Determines whether the x-axis scale is given in Wave-number (cm^{-1}) or Wavelength (nm).

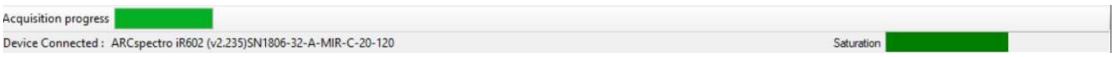


3.5 Status bars

On the lower left part of the console is an **Acquisition Progress** indicator.

On the lower right part of the console is a **Detector Saturation** indicator. It gives information on the signal level. If the indicator turns red the detector is saturated and the detector gain level or the light intensity have to be lowered.

Optimal signal levels:



The signal level varies between 100% and 10%

Saturation:

Either the detection gain should be decreased of or light level should be reduced.

Signal level is too low:

Detection gain or light intensity should be increased for optimal measurement performance.

If the Detection gain is changed, a click can be heard from the instrument, confirming that the operation was successful.

At the left of the bottom line the serial number of the actually used system is indicated.

3.6 Cursor Toolbar

The cursor toolbar allows showing cursors on the screen to compare measurement results and determine points of special interest. Cursors can be moved by click and drag either on the cursor position or on the lines that guide the eye. Cursors can be added and removed only when acquisition is switched off. Cursors stay visible when a new acquisition cycle is started. Values of actual cursor positions are shown. The screenshot below gives you and impression of the functionality.

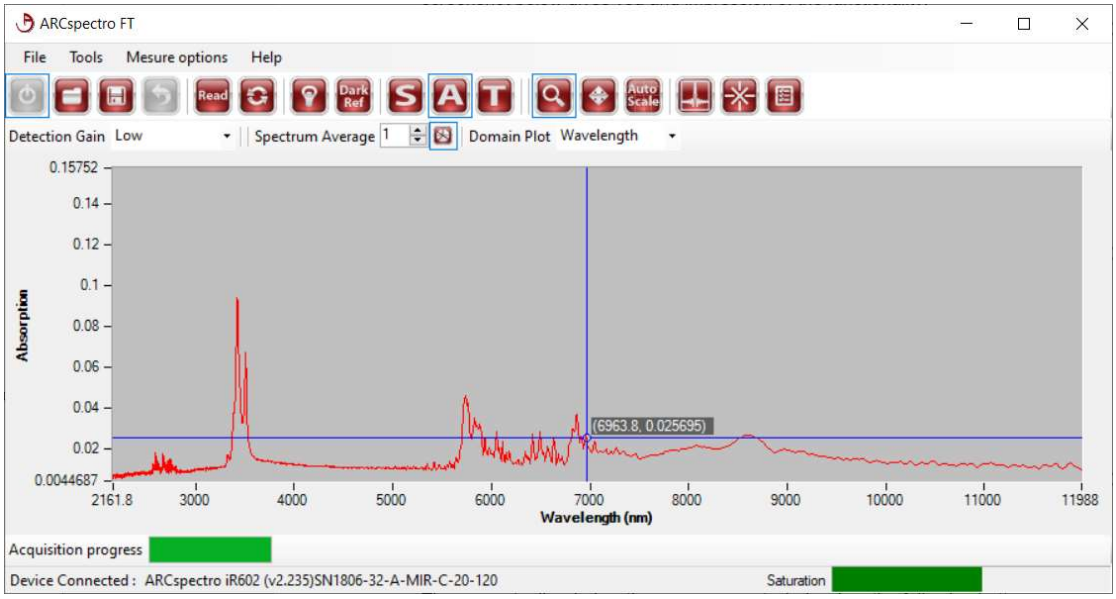


Figure 3-2 - Sample measurement with cursor toolbar and two cursors. The cursors can be moved by click and drag.

The cursor toolbar below the measurement window has the following buttons:

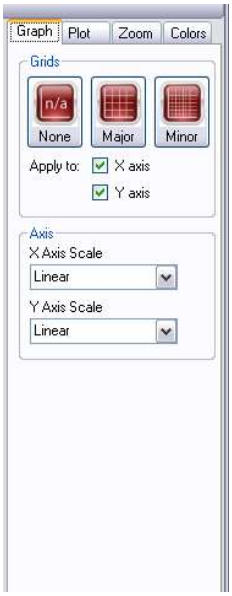
	**Add Cursor –** Activates a new curser.
	**Remove Cursor –** Re moves most recently activated curser
	**Remove Cursors –** Removes all cursers

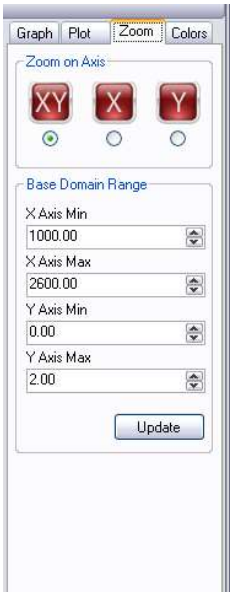
Note: Cursers cannot be moved when Zoom or Moving option are activated. Please deactivate this function to move cursers.

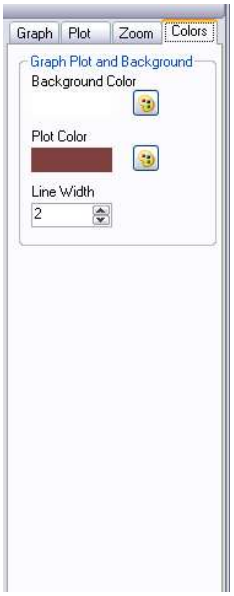
3.7 Graphing options

If you push the graphing option button  a side menu becomes visible on the right that allows you to change your graphing. There are four levels:

Graph Plot Zoom Colors







3.7.1 Graph

The graph submenu allows you to choose grids and to set linear or logarithmic scales.

	**None -** Removes the grid from the graph
	**Major -** Set a major grid.
	**Minor -** Set a minor grid.

The axis check boxes for x and y axis scale gives you the possibility to set the axis scale to predefined values (linear or logarithmic).

3.7.2 Plot

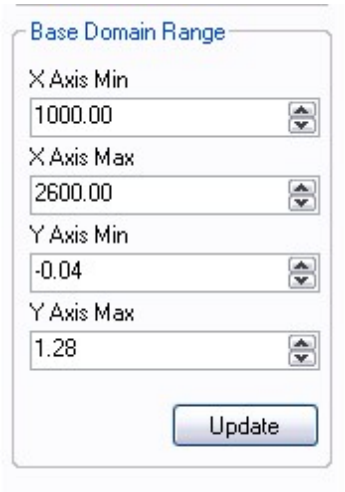
The plot submenu gives you the possibility to show the data points and to choose a convenient point size. In **samples** box you can switch on and off the sampling points and chose their point size.

3.7.3 Zoom on axis

The following functionality has to be used together with the zoom button  .

	When checked allows zoom in both axes.
	When checked allows zoom only in x axis
	When checked allows zoom only in y axis

The axis range can be set completely manually. In the box shown below axis parameters have to be given. Depending on the either wavenumber or a wavelength is chosen as “Domain Plot” option the values have to be wavenumber [per cm] or wavelengths [nm].



Please press update to activate new numbers.

3.7.4 Colors

Color submenu allows changing background color, plot color and line width for the screen. There are predefined values from which one can choose through scroll down menus.

CHAPTER 4 Measuring with the Arcspectro FT Rocket

4.1 Overview

The Arcoptix FT Rocket spectrometer is typically used to measure transmission spectra using a cuvette and a sample holder. This chapter describes the general approach to collecting data and presents a series of suggestions to optimize the quality of measurement. Since the spectrometer can measure the spectrum of a broad range of samples in a large number of applications, the information presented in this chapter is somewhat general in nature. The analyst will likely find specific information about sampling and collecting spectra for the specific sample in the general scientific literature.

A cuvette and a sample holder are used when the spectrum of a liquid is to be obtained. The standard cuvette has a 1 cm path length (although other lengths may be used) and requires approximately 2 mL of sample. If the available sample is less than 2 mL, a number of smaller cuvettes are available and an adapter can be used to reproducibly position the cuvette.

NOTE: It should be noted that the absorbance of a sample is proportional to path length, and using a thinner cuvette will be beneficial for samples with large absorbance values.

The cuvette is an integral part of the optical system, and should be handled with care. The following points should be noted to ensure the fidelity of collected spectra:

- In case of a transmission measurement with cuvettes: always place the cuvette in the light path so that the same wall plane faces the incoming light to ensure a constant path length.
- Do not get fingerprints on the optical faces of the cuvette. If you accidentally touch an optical surface, wipe it off with a lint free tissue saturated with methanol and allow the methanol to evaporate.
- If an optical surface of the cuvette is scratched, chipped or becomes cloudy, position the cuvette in the sample holder so that the light does not go through that surface.
- The sample should be dissolved in a suitable solvent and should be homogeneous. Spectroscopic grade or other highly purified solvents should be used whenever possible. If the source of the solvent is changed, verify that the new solvent and the old solvent are equivalent and collect a new background spectrum. If the sample contains particulate matter, make sure that it is filtered to remove the solid material. If there are air bubbles in the sample, remove them before taking a measurement. Air bubbles are occasionally observed in aqueous samples that have been allowed to sit undisturbed for a period of time.

4.2 To collect a spectrum

Install the hardware system correctly by connecting fibers properly and switch on the source. Connect the spectrometer and start the software. Adjust the intensity and the detection gain to operate in the optimal range. A Halogen lamp of sufficient power is recommended for operation. Click on “Read”  to start an acquisition. Figure 4-1 below shows you a sample measurement in the wavelengths domain. Data are collected in 2.5s, but the measurement takes typically 1.5s more because of additional signal processing that has to be performed. If the option “show interferogram”  is activated, the interferogram related to the spectra is also shown.

Figure 4-1 - Spectrum and corresponding interferogram (IGM)

After a measurement has been performed the scale in the graph can be eventually arranged. To do so, press the Auto-Scale  button.

To get access to functionalities like absorption and transmission measurements, you need to measure a **reference spectrum**. Place a reference sample (it is often just an empty cuvette) in the sample holder and collect the background (baseline) spectrum. To do so, perform a measurement with “Read”  and then press the “Set baseline spectrum” button  . The following functions get accessible (highlighted):  Spectrum,  Transmission,  Absorption.

Measure the reference sample again in transmission mode ( ). The result will be a transmission value of 1, apart from measurement noise, all over the usable wavelength range, as shown in Fig. 4 - 4 below.

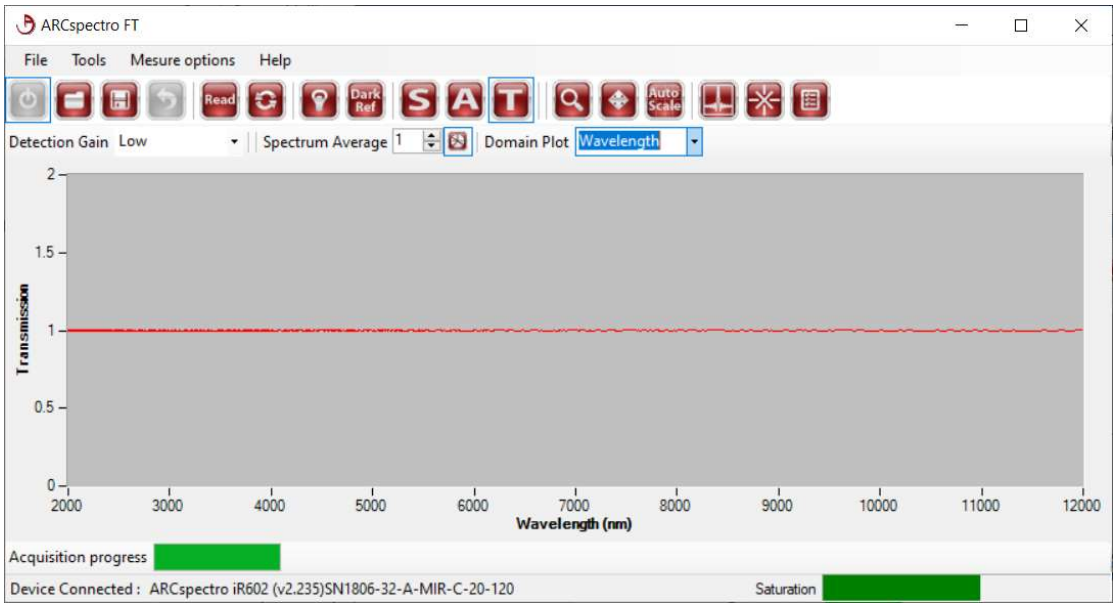


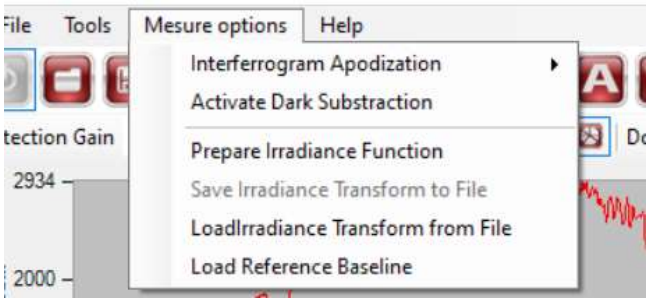
Figure 4-2 – Checking the noise level in the baseline

NOTE: If appropriate, the background spectrum can be taken using an empty cuvette.

The spectrum of a standard should be collected on a periodic basis (in many laboratories, a sheet of a polymer is employed as a standard). The standard should have a number of absorbance bands spread across the spectral region. When the spectrum of a standard is collected, the analyst should check that the intensity of the bands and the wavelength remains constant over time.

4.3 Advanced Features – Measure Options Menu

The software offers some advanced options that are both accessible using the Measure Options Menu. Before using these options, make sure that you understand what they do by reading the following paragraphs.

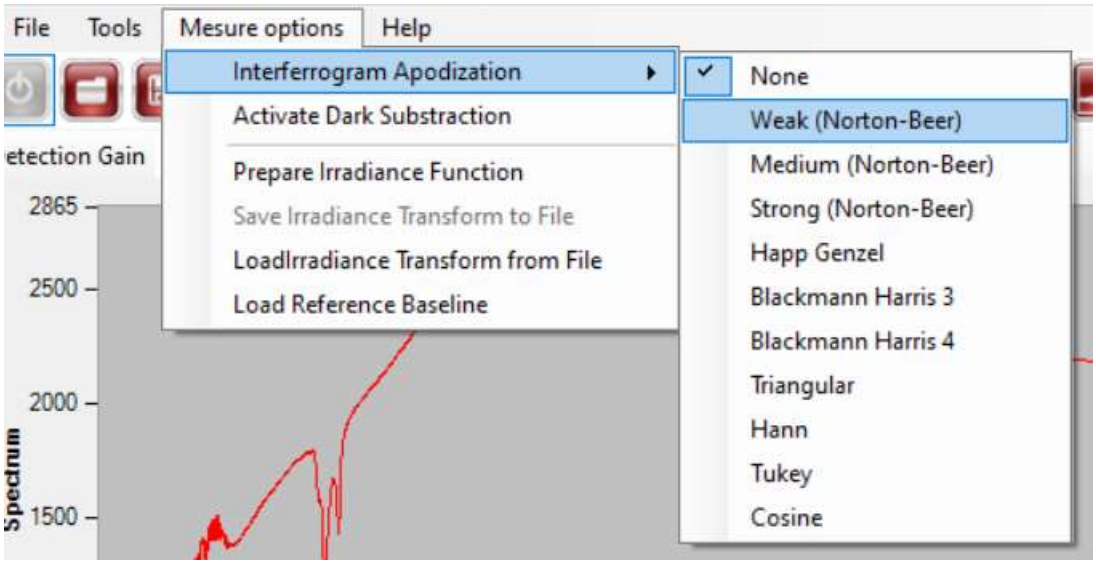


4.3.1 Interferogram apodization

The spectrum that is produced by the software is, by default, produced by Fourier transformation of the unapodized interferogram (None).

This Interferogram Apodization option allows you to apply a Weak, Medium or Strong **Norton-Beer** type apodization (and some others) to the interferogram before the Fourier transformation. The main effect of Interferogram Apodization is to smooth the spectrum. It can also eliminate ripple effect on the spectra. Finally, it may also enhance the linearity of absorption measurements if narrow bands are present such as in gases.

Generally, we recommend to work with Norton-Beer weak apodization.



As for the Interferogram Averaging, a clear and visible interferogram center burst must be available for the method to operate effectively. When measuring very weak signals or narrow spectra, set the apodization to None.

4.3.2 Dark Substration

One particular advantage of Fourier-transform spectrometers over dispersive instruments is that detector dark current signal is not producing any dark (offset) spectrum. This is because only the AC components of the detector signal (the interferogram) are carrying spectral information.

In certain specific situations, a dark background signal may be present. In this case background subtraction may be needed. For example, when connecting an internally illuminated integrating sphere, some light is sent to the spectrometer even when no sample is placed on the measurement port, as shown on Figure 3 - Dark signal measured with an internally illuminated integration sphere

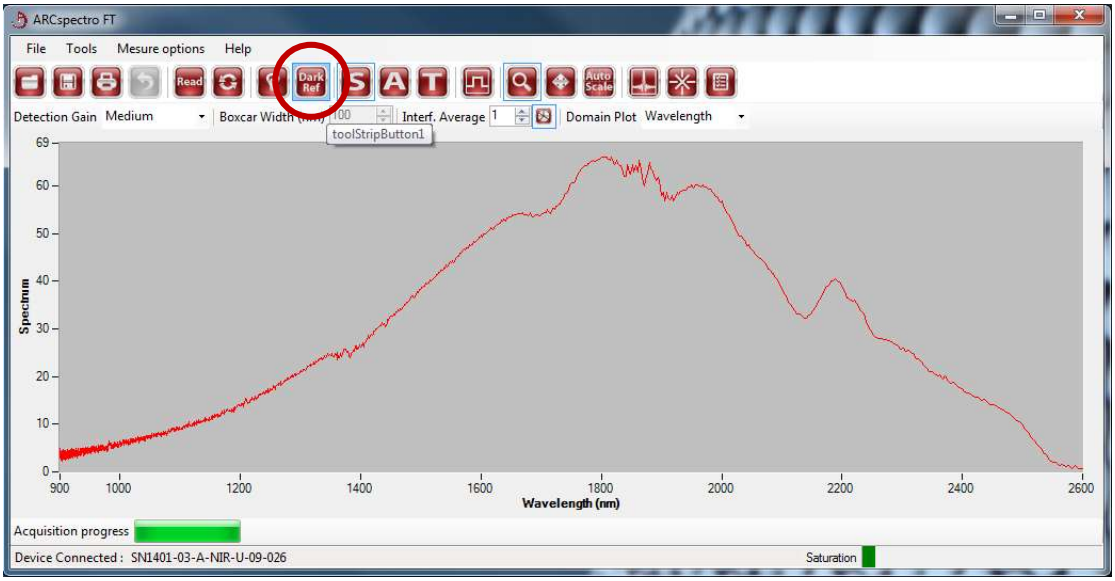


Figure 3 - Dark signal measured with an internally illuminated integration sphere

Press the ***Dark Reference*** button 

to store this measurement as the dark spectrum. Then go into the ***Measure Options*** menu and activate the Dark Substraction option. The software will now substract the Dark Spectrum from the next measured spectra
You can now proceed as usually by measuring the (white) baseline reference spectrum and then switch to any measurement mode (transmission, absorption).

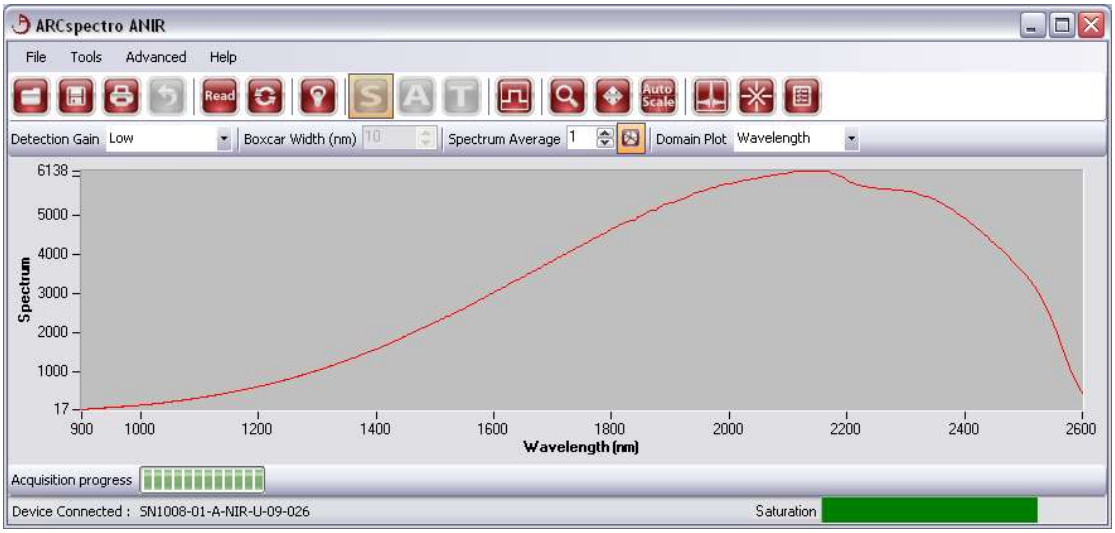
4.3.3 Irradiance calibration

The Arcspectro software disposes of an interface for calibrating the spectrometer for irradiance measurements. In order to perform such an irradiance calibration, the user needs:

- A calibrated light source

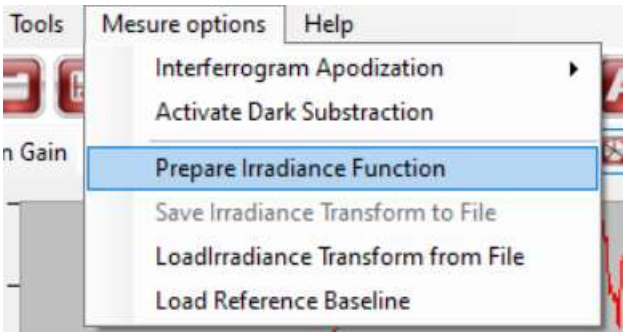
- A data file containing the irradiance values of the calibrated light source at wavelengths between 900 and 2600nm (or the equivalent wavenumbers).
-

Connect the calibrated light source to the spectrometer and tune the light intensity and gain level to obtain a satisfying signal level.

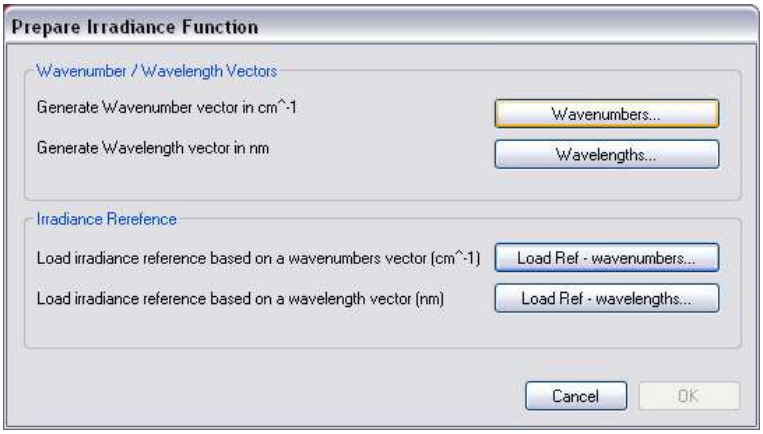


NOTE: performing averaging (either by spectrum or interferogram averaging) in this measurement is strongly advised to reduce noise, as noise in the light source measurement will propagate as fixed pattern noise to subsequent irradiance measurements.

In the Advanced menu, select *Prepare Irradiance Functions*:

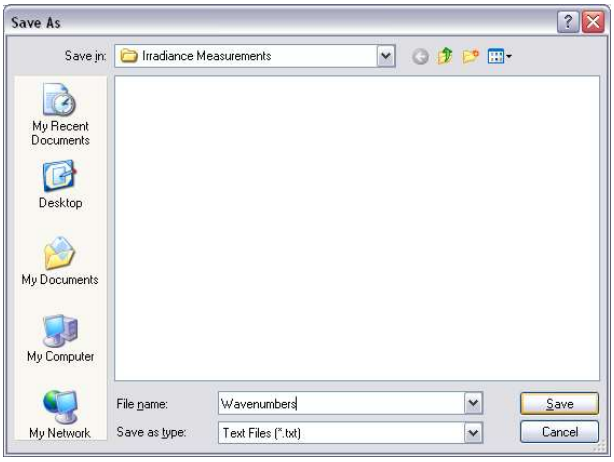


This will open a new window interface helping you to prepare irradiance data:

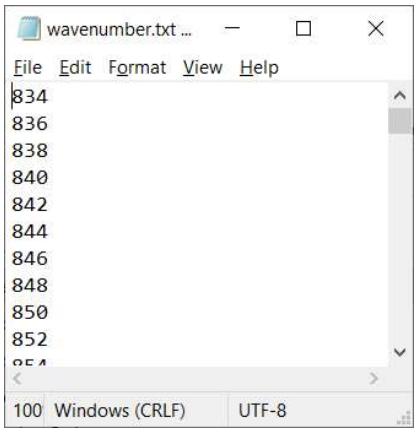


The upper part of the window, *Wavenumber/Wavelength vectors,* allows you to generate text-format files with the internal Wavenumber (or Wavelength) grid, while the lower part , *Irradiance Reference,* allows you to load data into the system.

The calibration procedure can be realized either in wavenumbers or in wavelengths. Pressing the *Wavenumbers* button in the *Prepare Irradiance Function* window will open a dialog to save a file:



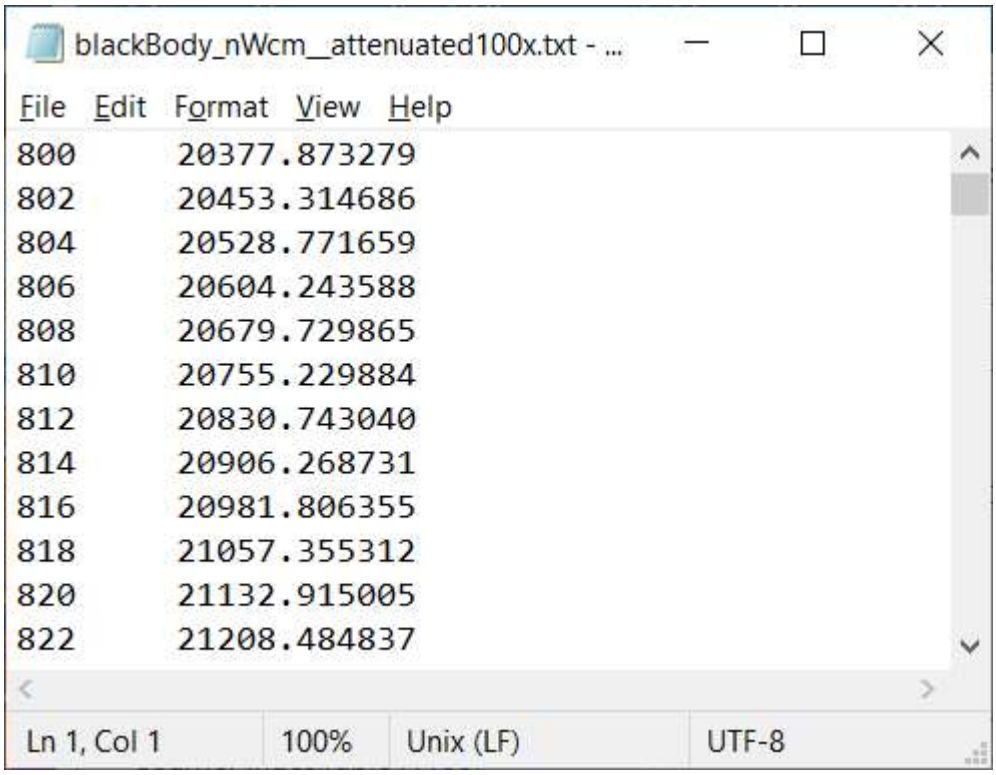
The content of the file are wavenumbers in the units of [cm^{-1}]:



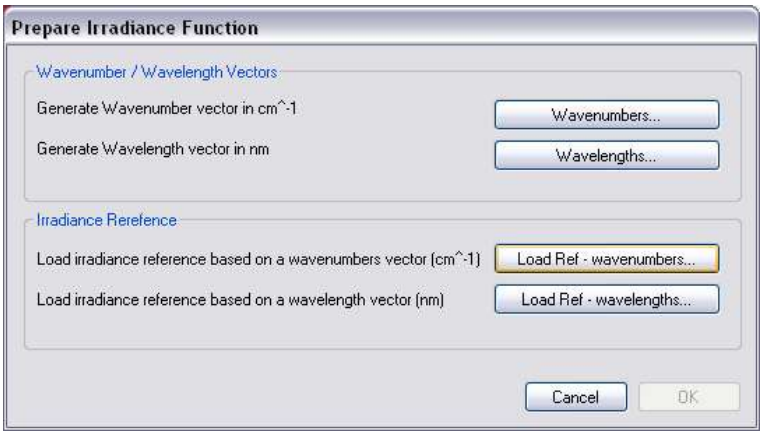
Note that a similar file can be generated with wavelengths in the units of [nm] by pressing the *Wavelengthss* button in the *Prepare Irradiance Function* window.

NOTE: due to the Fourier-transform functioning principle of the Arcspectro FT ROCKET, the generated wavenumber vector is equally spaced but the wavelengths vector is not.

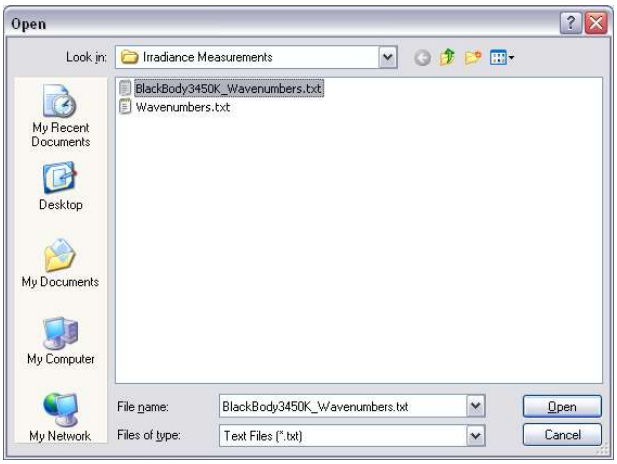
In order to calibrate the spectrometer for irradiance measurements, the user needs to interpolate irradiance data from the calibrated light source data file onto the wavenumber (or wavelength) vector in the file just generated, with the help of an external program (e.g. EXCEL or MATLAB). Then a text file must be generated with two-columns [Wavenumber Irradiance] **separated by a tab character** as in the following example:



Once the two-columns text file is ready, go back to the *Prepare Irradiance Function* window and press the *Load Ref – wavenumbers* button (or *Load Ref – wavelengths* button if you prepared a reference file based on wavelengths).

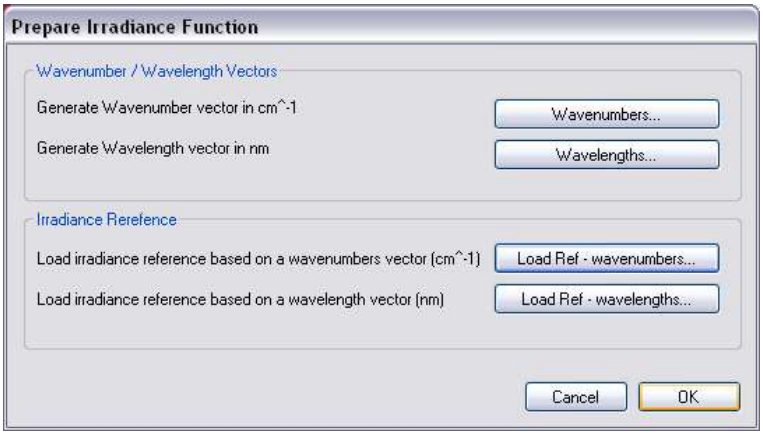


In our example, we prepared a two-column file called *BlackBody3450K_Wavenumbers.txt* :



Choose the file and press *Open*.

Once the file is loaded, you are allowed to press the *OK* button to validate the calibration:

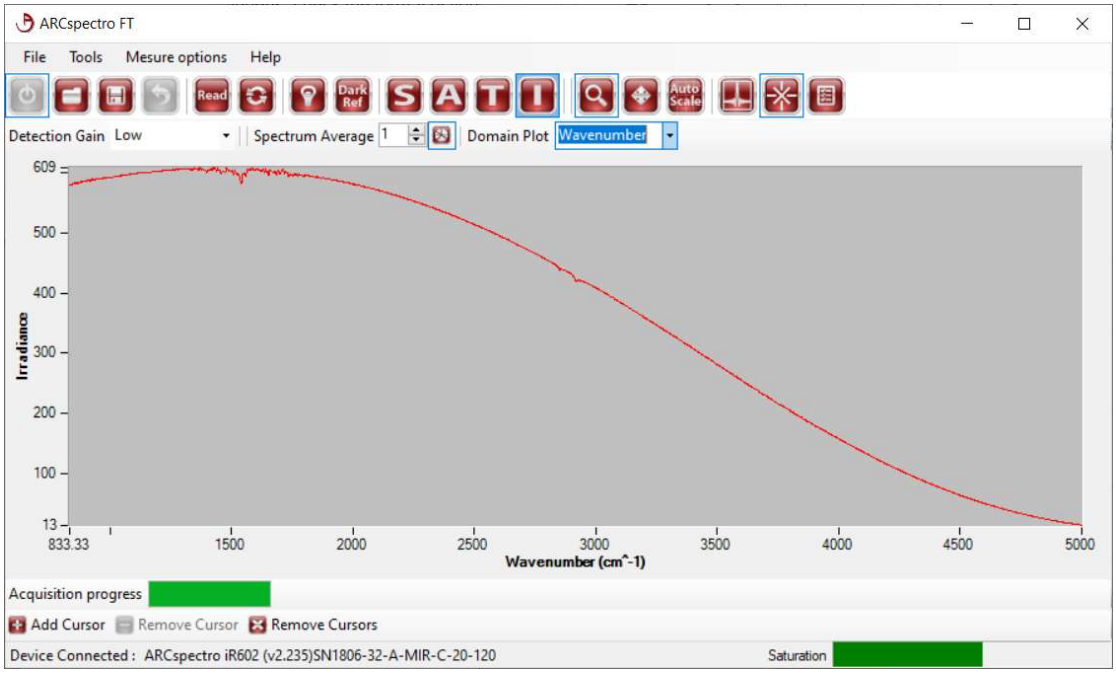


IMPORTANT NOTE: interpolating the irradiance data onto the spectrometer wavenumber (or wavelength) vector is NOT made internally by the Arcspectro software, as this procedure may differ depending on the resolution of the irradiance data file thus requiring expertise by the user.

If you try to load a file with wavenumbers (or wavelengths) differing from the required ones, the system will display the following error:

If this happens, check the format of your file and the wavenumbers (wavelengths) data and try loading it again.

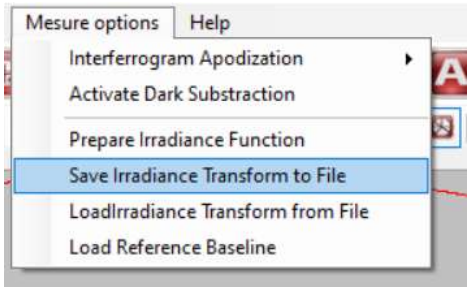
Back in the main GUI window, a new button  will appear in the Tools bar. Click on it to display irradiance values.



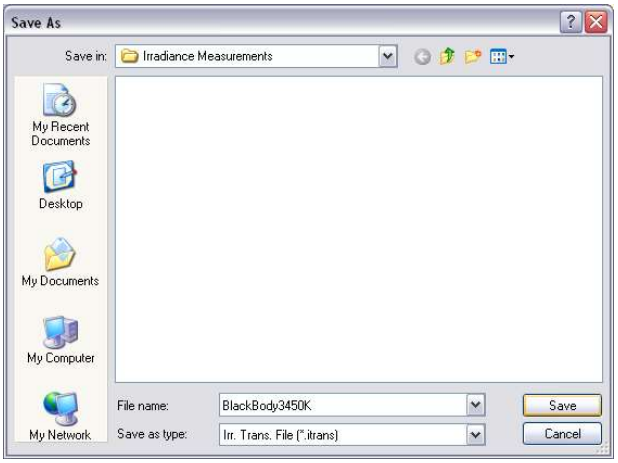
Now you can perform irradiance measurements by pressing the read button  .

Saving and reloading Irradiance calibration files

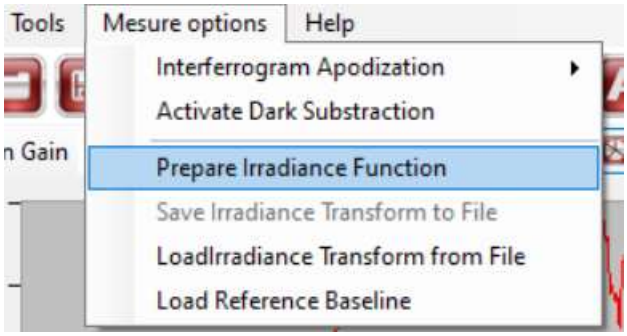
Once you have completed the irradiance calibration, the result can be saved and reloaded for further use. To save calibration data, select *Save Irradiance Transform to File* in the *Advanced Menu*:



This will open a dialog window for saving the calibration in a **.itans* file.



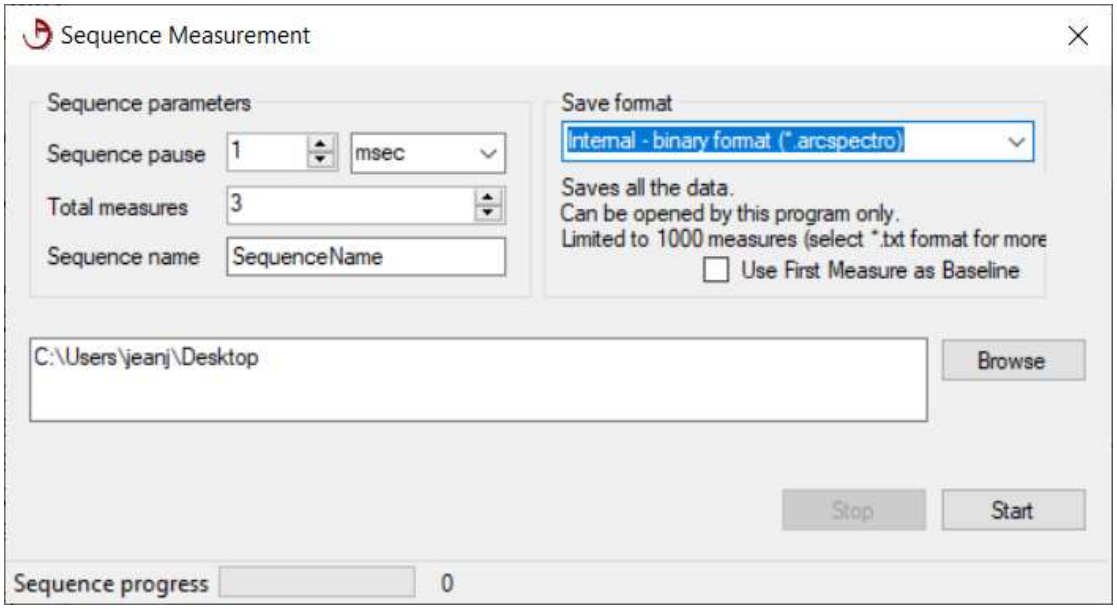
To reload the calibration, select Load Irradiance Transform from File in the Advanced Menu:



NOTE: Modifying the coupling optics from the light source to the spectrometer (e.g. changing the fiber or focusing optics) is likely to alter the spectrum entering the spectrometer, thus invalidating the irradiance calibration.

4.3.4 Sequence measurement

The Arcspectro software allows you to save a time-series (sequence) of measurements. To keep operation flexible, the feature allows saving data in two different formats. The functionality is accessed via the Tool menu that allows opening two windows.



Sequence measurement allows choosing the total number of measurements, the delay between measurements and a sequence name. “Sequence pause” can be given in milliseconds (msec), seconds (sec), minutes (min) and hours.

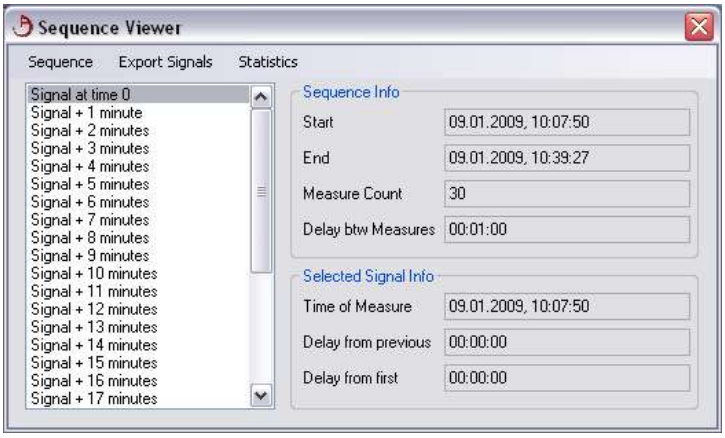
NOTE: The acquisition time is not counted in the “sequence pause” parameter. You will add the measurement time (which depends of the computer and resolution of the device).

The save format scroll down menu gives to options for saving: Binary Format or text format. If you want to use the data outside the measurement program for further processing you should use the option Spreadsheet-text format.

A box in the save format area allows you save the first dataset as baseline. If not checked the internal reference as set before by the baseline measurement button will be saved with the data.

You have to give a sequence name and specify the path where the date should be saved. There will be an automatic numbering of the file names. If text format is used, the time when the measurement was performed is part of the file name and all data are saved in text format that can be read with compatible programs like EXCEL or MATLAB.

If a sequence is saved in binary format it will be available for further processing. Choosing in the **Tools** menu the option Sequence viewer opens a standard Windows dialog box that allows you to load a sequence. Note, only binary data can be loaded. Choose your measurement sequence and confirm with OK. The data will be shown in the active window. It might be necessary to rescale the graph. At the same moment, the following screen will appear. It gives an overview over the recorded sequence and allows saving selected data into spreadsheets via a scroll down menu.



The spectrums are listed in the box at the left side of the Viewer Window. The upper right side displays some relevant sequence information and the lower right side shows signal-specific information.

Use the Open option in the **Sequence** menu to open a new sequence. The Clear option of the same menu clears all the displayed sequence spectrums.

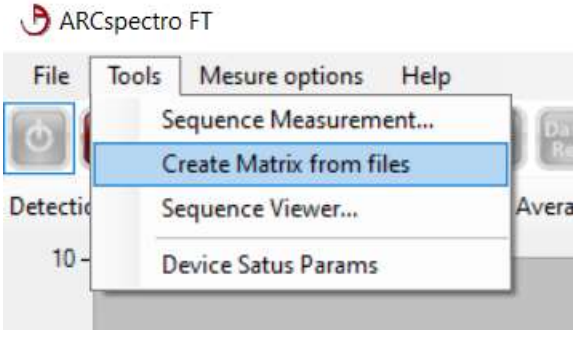
You can export a selected signal to a spreadsheet format using the Export Selected Signal to Spreadsheet option of the **Export Signal** menu.

Finally you can display an average of the sequence spectrums by checking the Plot Average option in the **Statistics** menu. The average spectrum will be displayed on top of the sequence signals with yellow squares. The following figure illustrates 10 consecutive measurements of a 1500nm long-pass filter.

Creating a Matrix of measurements from files

It is possible to make a txt file where a group of selected measurement are concatenated together in a tab separate txt file. Such files may be used for importing the measurements in a separate third-party analysis program.

First, select the *Create Matrix from files…* option in the Tools menu.

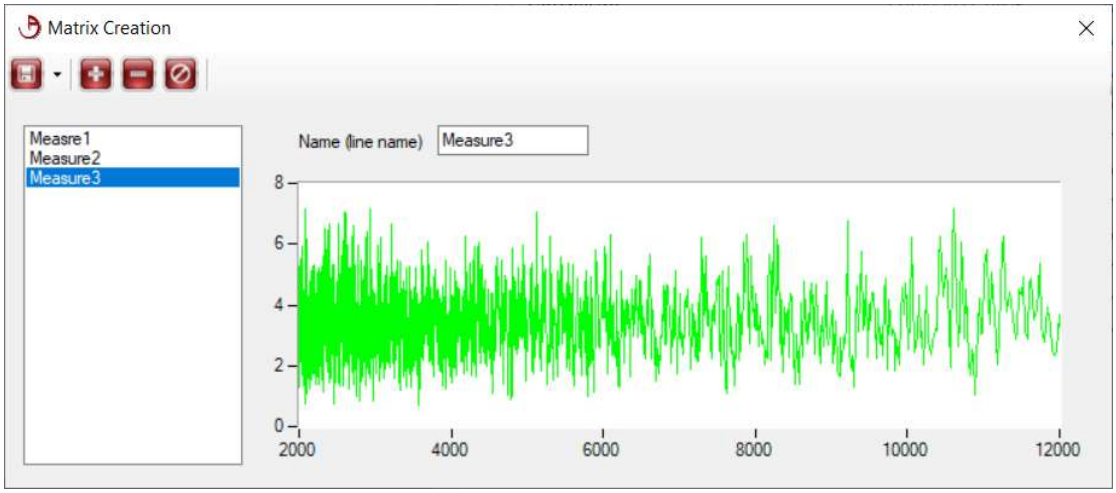


This option brings up the following dialog box.

You can add the signals you want to export using the *Add Signal* button. You can keep the dialog box open as you make a measurement then add the resulting signal, make another measurement, add it and so on. You can always select and view a signal

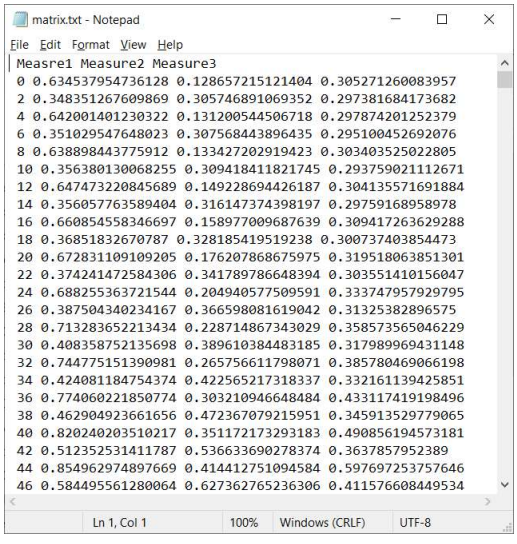
before saving the matrix to a file (using the *Save File* button) and you can also delete a selected signal or clear the whole list using either the *Remove Signal* or *Clear all Signals* buttons.

This is what the dialog box looks like after having added 3 signals:



You can select the signals using the left-sided list box. Doing so shows a preview of the signal in shown in the graph. You can change its name in the *Name (Line name)* textbox if so desired.

When all the desired measurements are loaded in the list, you can press the save button and save all the measurement together in a tab separated matrix. The saved file is a TXT format file as shown here below:

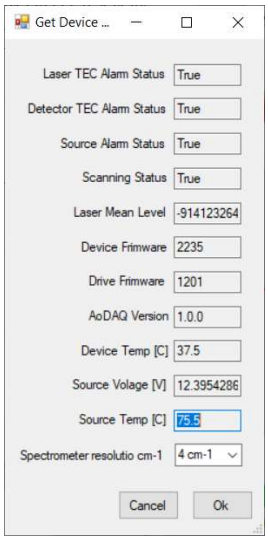


First column is the wavenumber and the following columns are the measurement “Measure1, “measure2”, “measure3”,….

This Txt file may be handy for exporting your measurement results to another program for analysis.

4.3.5 Device status

The device status window permits to have an overview of the general hardware status and parameters of the device:



- Laser TEC Alarm: indicates if the temperature of internal control laser is on target
- Detector TEC Alarm: indicates if the temperature of the detector is on target.
- Source Alarm Status: indicates if the source is ok (or maybe broken) (if installed)
- Scanning Status: indicates whether the interferometer is scanning correctly
- Laser mean Level: indicates the intensity level of the control laser
- Device, Drive and AoDAQ versions number indicates which versions of drivers and software is installed in the device.
- Device temperature indicates the temperature on the electronic board next to the interferometer (should not exceed 50 °C)
- Source voltage: Voltage on the source (if installed)
- Source Temp: temperature of the source electronic board.

Notice that the values indicated are sometimes misleading and not always useful. This is mainly for servicing purposes and sometimes debugging or repairing purposes.

4.4 Quantitative Measurements

The **transmission** (T) of a sample is defined by:

$$T = \frac{I}{I_o}$$

where I is the power of the light that is transmitted by the sample, I_o is the power of the light incident on the sample.

The **absorbance** (A) of a sample is the logarithm (base 10) of the reciprocal of the transmittance:

$$A = -10log_{10}T = 10log_{10}\frac{1}{T}$$

Beer's Law, can be used to determine the concentration of the compound of interest.

$$A = acL$$

where: A is the absorbance, a is the molar absorbance coefficient, which is a constant for a compound in a given solvent at a given temperature, c is the concentration of the compound L is the sample thickness.

CHAPTER 5 Troubleshooting

5.1 Sample Related Spectra Issue

If the instrument appears to be working in an acceptable manner (e.g. the spectra of the standard is acceptable) and unacceptable sample spectra are obtained, it is probable that the difficulty is related to the sample. Typical sample related issues are indicated in the following Table:

Sample Related Issues

Problem	**Cause**	**Solution**
The absorbance is weak or % T is very high (noisy spectrum)	The sample is too thin or too much light is lost	In transmission use thicker samples
		Increase the number of averages in order to increase the SNR
The absorbance is too strong or % T is near zero	The sample is too concentrated or thick	Dilute the sample or use a thinner sample. Sometimes an ATR measurement may help (low penetration).
Intensity of peaks or signal vary in time.	Sample variation (evaporation) or temperature variations. Fiber vibrations or displacement,	Control the temperature or make baseline and sample measurement as close as possible in time. Control that vibrations are not present (like ventilator running on the table)
Reproducibility	Temperature variation, Sample variation, setup variation (particularly with fibers)	Variation of a percent are common when doing spectroscopy.

5.2 General troubleshooting

Since the Arcspectro FT ROCKET is employed in a system that includes a light source, a sample probe and a sample, all troubleshooting activities should include all components of the system. Troubleshooting can be simplified by a consideration of the following guidelines.

In principle the light source can easily be check by bear eye. Sample probe and sample can be the cause of the problem but the variety of samples and measurement methods are so large that we will not discuss this here.

First of all, as for many device, a switch off and switch on followed by a restart may solve the problem. Also some software bugs that are related a to a particular combination of operations are not excluded. If an error message is presented, press the **Continue** button indicated on the *Error Message* dialog box. If this does not remedy the problem, turn off the spectrometer, disconnect the USB cable, reconnect and restart the software.

If the error persists (and you can still connect to the spectrometer, you may have a look at the device status windows (see in the manual). Alarms (first 3 items in the list) should be false, Scanning Status value should be true, Laser mean level around 10 Exp 7 (however this value is variable from device to device and may be also at 10 Exp 6), Device Temp (below 60°). Other values are not relevant for all devices.

Run a standard (or a series of standards) on a periodic basis to verify that the system is performing properly. When abnormal data is obtained, collect the spectrum of a standard and compare the spectrum to one that was previously obtained.

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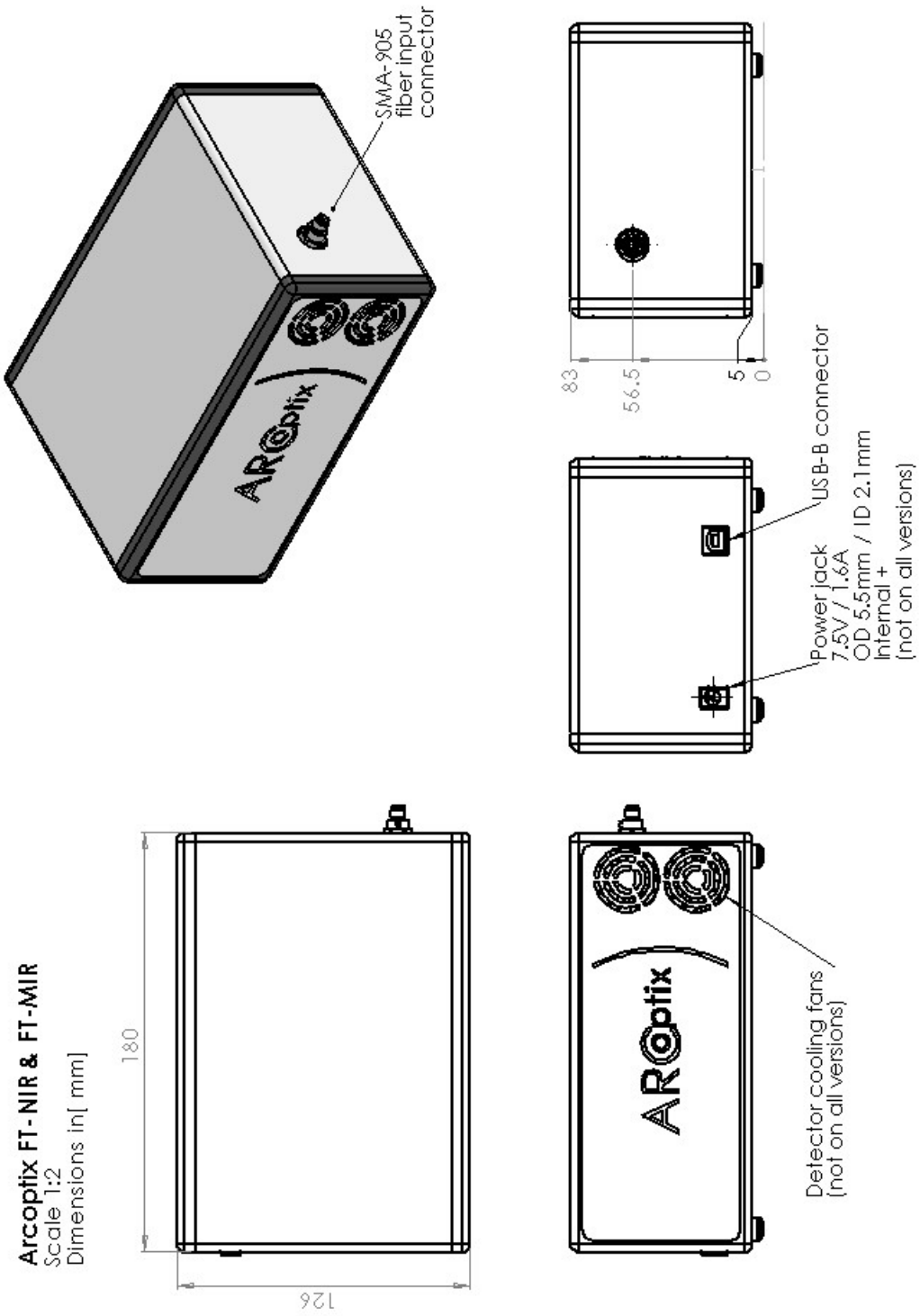
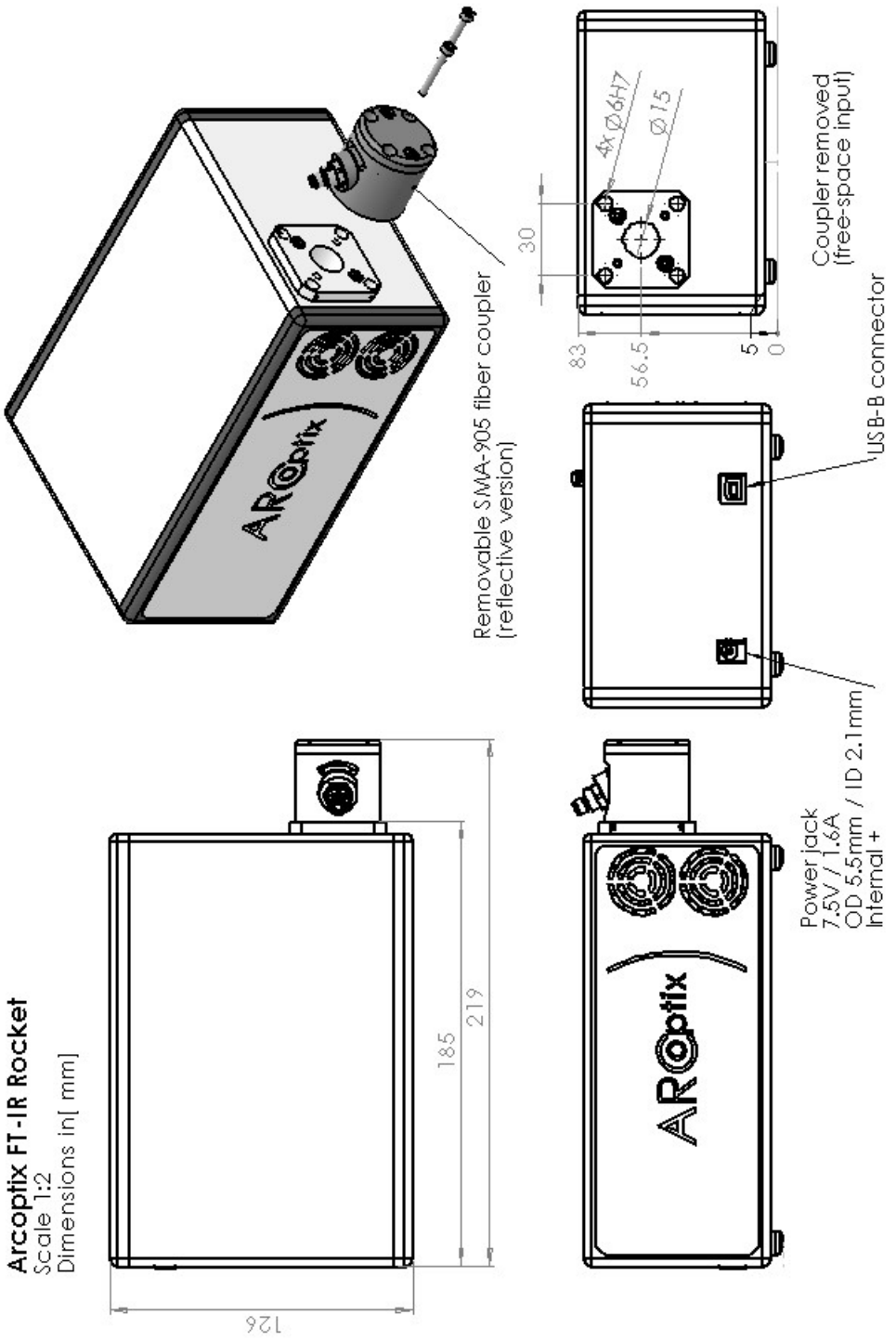
Symptom	Cause	Solution & Checks
Cannot connect (offline)	USB cable is loose, Reset port problem, Driver problem spectrometer problem. AODaqwin.exe server did not start in background	Check cables for good contact. Rest the computer (sometimes for portables remove the battery a few seconds). Check driver in device manager. Check in Task manager in the AOdaqwin.exe serveur is starting in bakground
No signal or only noise	Problem with setup (make a standard measurement). Problem with light source, problem with the detector or internal control laser	Make a simple standard measurement where all the other parameters are sure and known. Check lase level in device params. Restart software, spectrometer and computer.
A lot of variation or drift in the signal	Thermocooler defect, or internal control laser. Setup problem. interferometer misaligned.	Check Alarms in the device status. Check reproducibility with a simple setup.
Wavelength Shift	In principle not possible	Contact arcoptix
Strange signal	Detector saturated or not enough signal. Defect laser. Or interferometer misaligned.	Contact Arcoptix or its local representative. Check with a simple setup the results.
Strong water vapor lines	desiccant saturated	Replace desiccant.

Appendix 1 – Dimensions

FT-NIR & FT-MIR (fiber input)

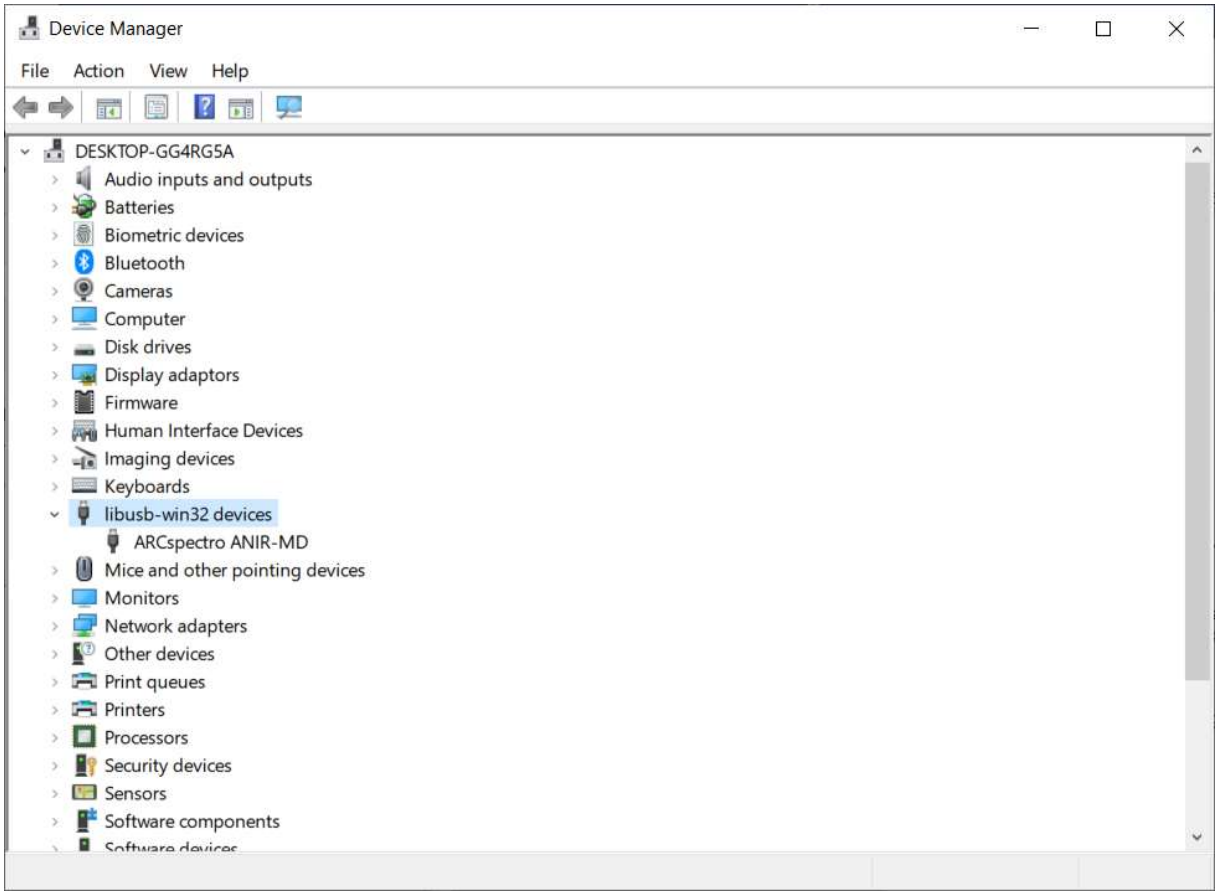



Arcoptix FT-IR Rocket
Scale 1:2
Dimensions in[mm]
126
185
219
ARCoptix
Removable SMA-905 fiber coupler
(reflective version)
4x Ø6H7
Ø15
30
83
56.5
5
0
Coupler removed
(free-space input)
USB-B connector
Power jack
7.5V / 1.6A
OD 5.5mm / ID 2.1mm
Internal +

Appendix 2 – Installation

Use the provided installer file “ARCspectroRocket 3.X.Y Installation Package.exe” to install the new software. The installer will also install the USBLIB driver.

Once the software installation is complete, re-connect the spectrometer and open the Device Manager to check if the “ARCspectro ANIR-MD” is properly recognized as “libusb-win32 devices” as shown below.



Now you can start the new ARCspectro Rocket software to control the spectrometer.